Warning: May contain chemistry…

And cats.

And drawings which demonstrate that I should not give up my day job to become an illustrator

Recent advances in Perovskite solar cells

Nov 17, 2018

Science Circle

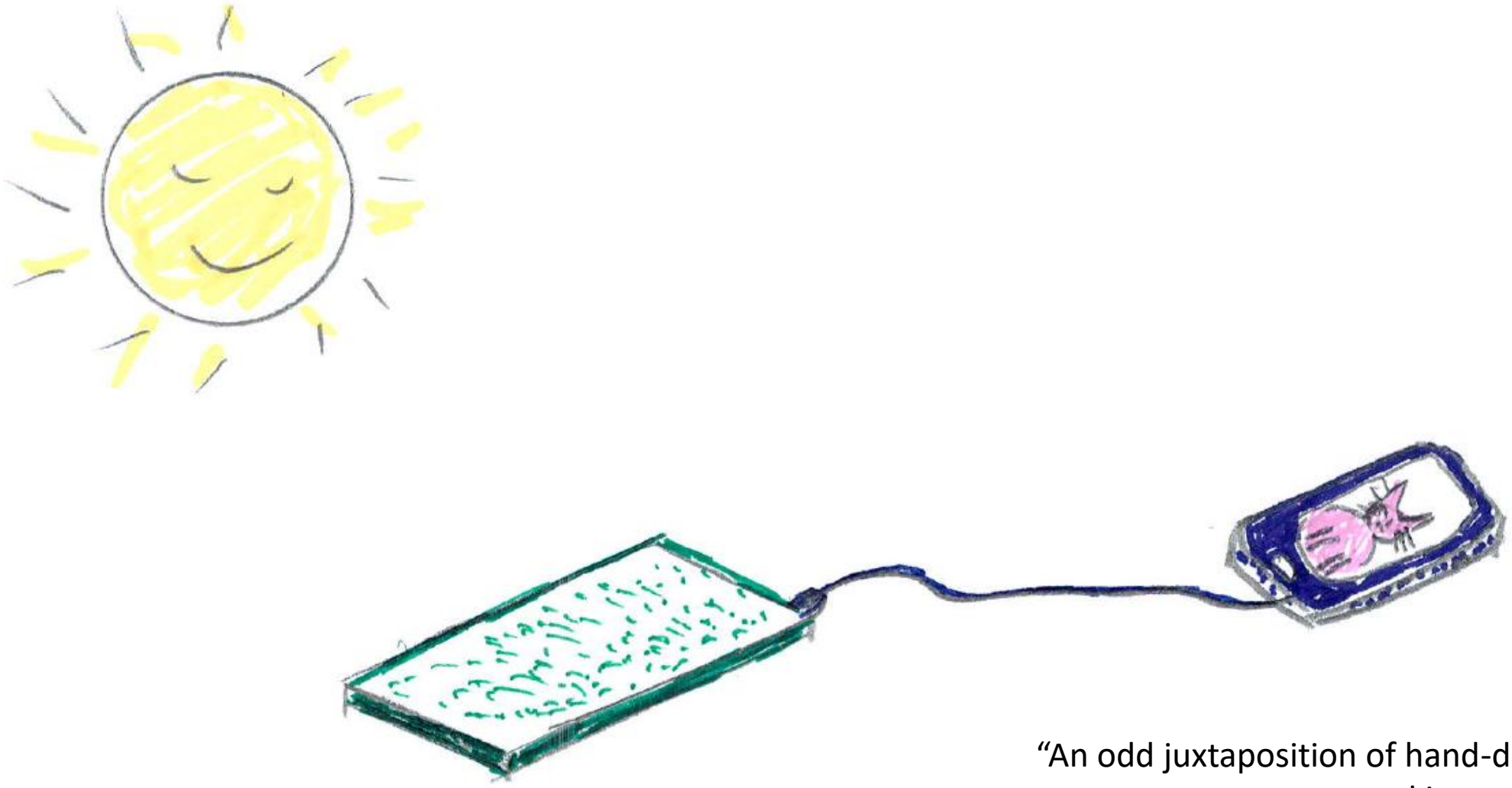
Mike Shaw

Dr. Michael J. Shaw

Dist. Res. Professor of Chemistry,

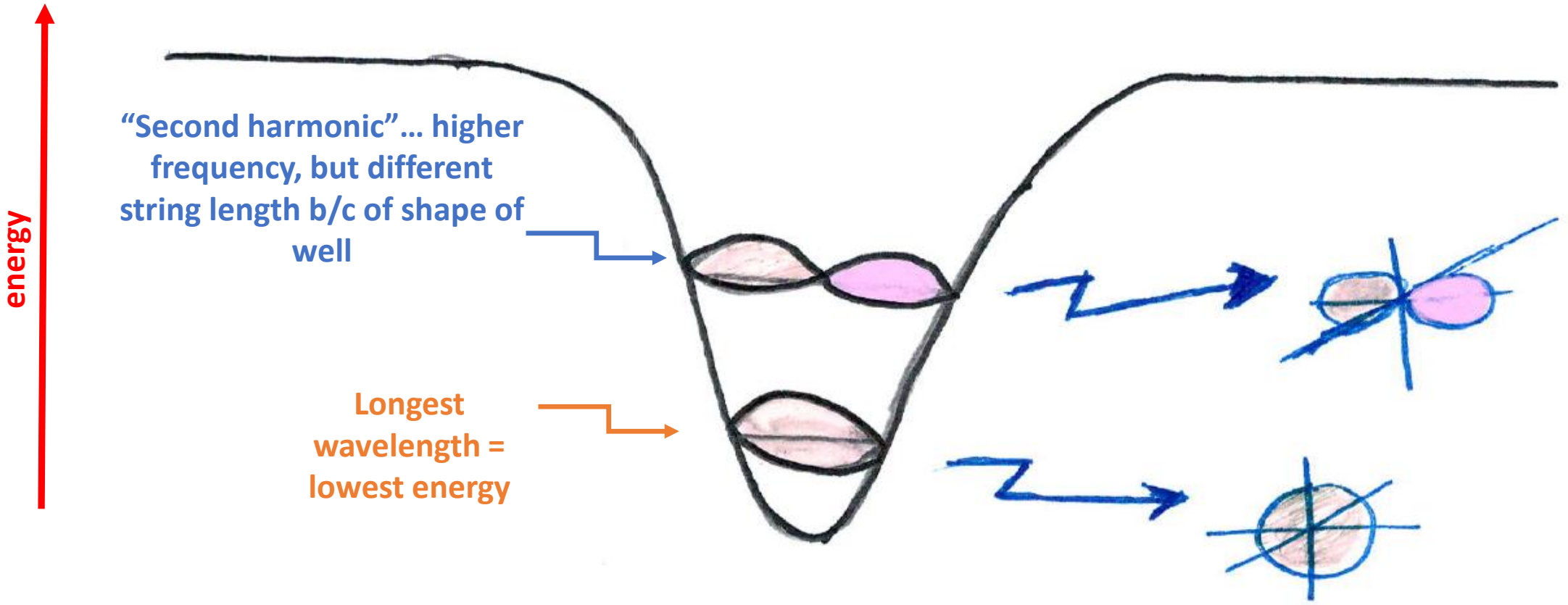
Southern Illinois University Edwardsville

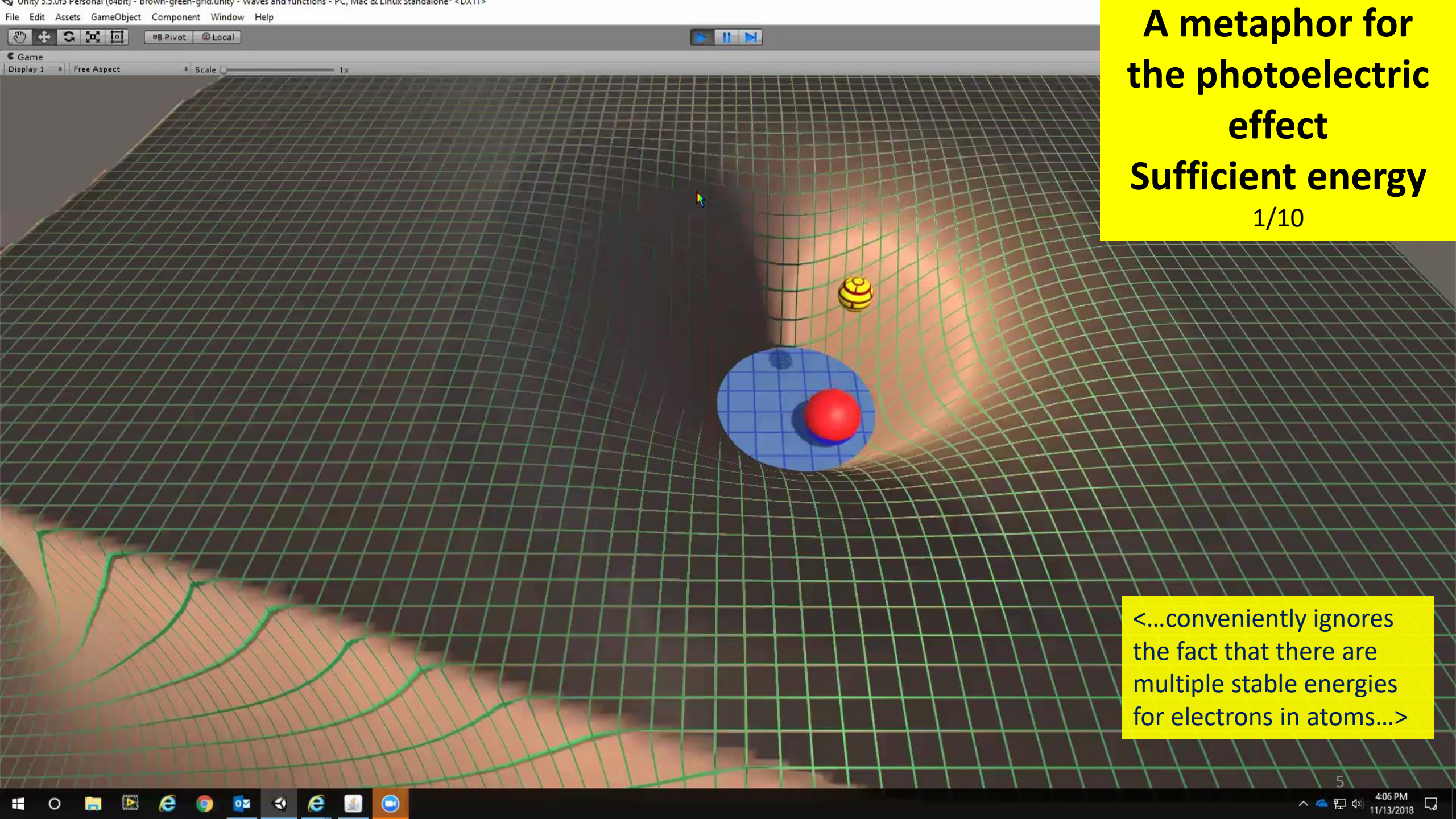
So how does solar power work?



"An odd juxtaposition of hand-drawn and computer-generated images…."

Let's talk about how electrons interact with nuclei… Vibrations on a string?

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A metaphor for the photoelectric effect
Sufficient energy
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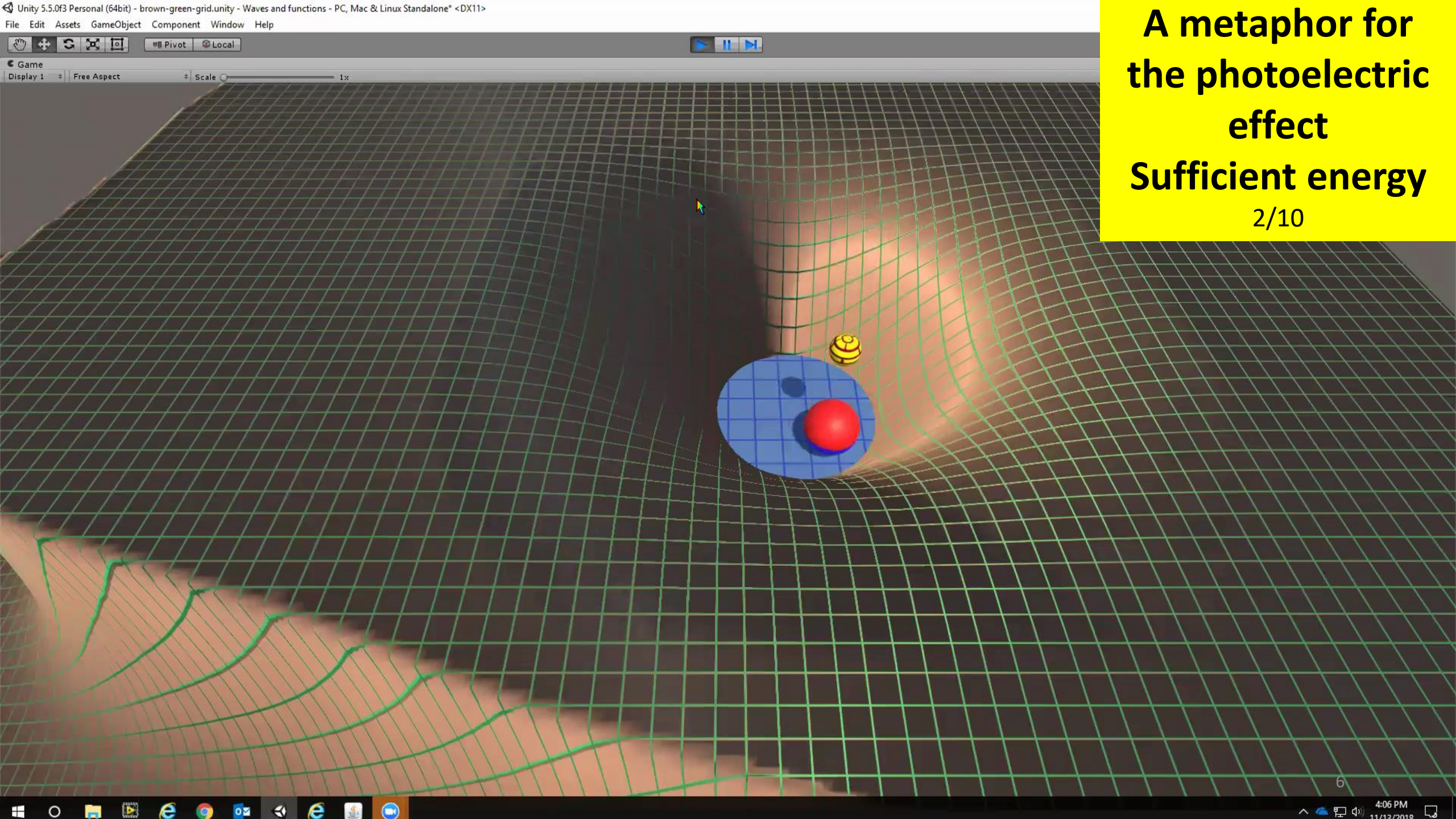
<…conveniently ignores the fact that there are multiple stable energies for electrons in atoms…>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A metaphor for the photoelectric effect
Sufficient energy
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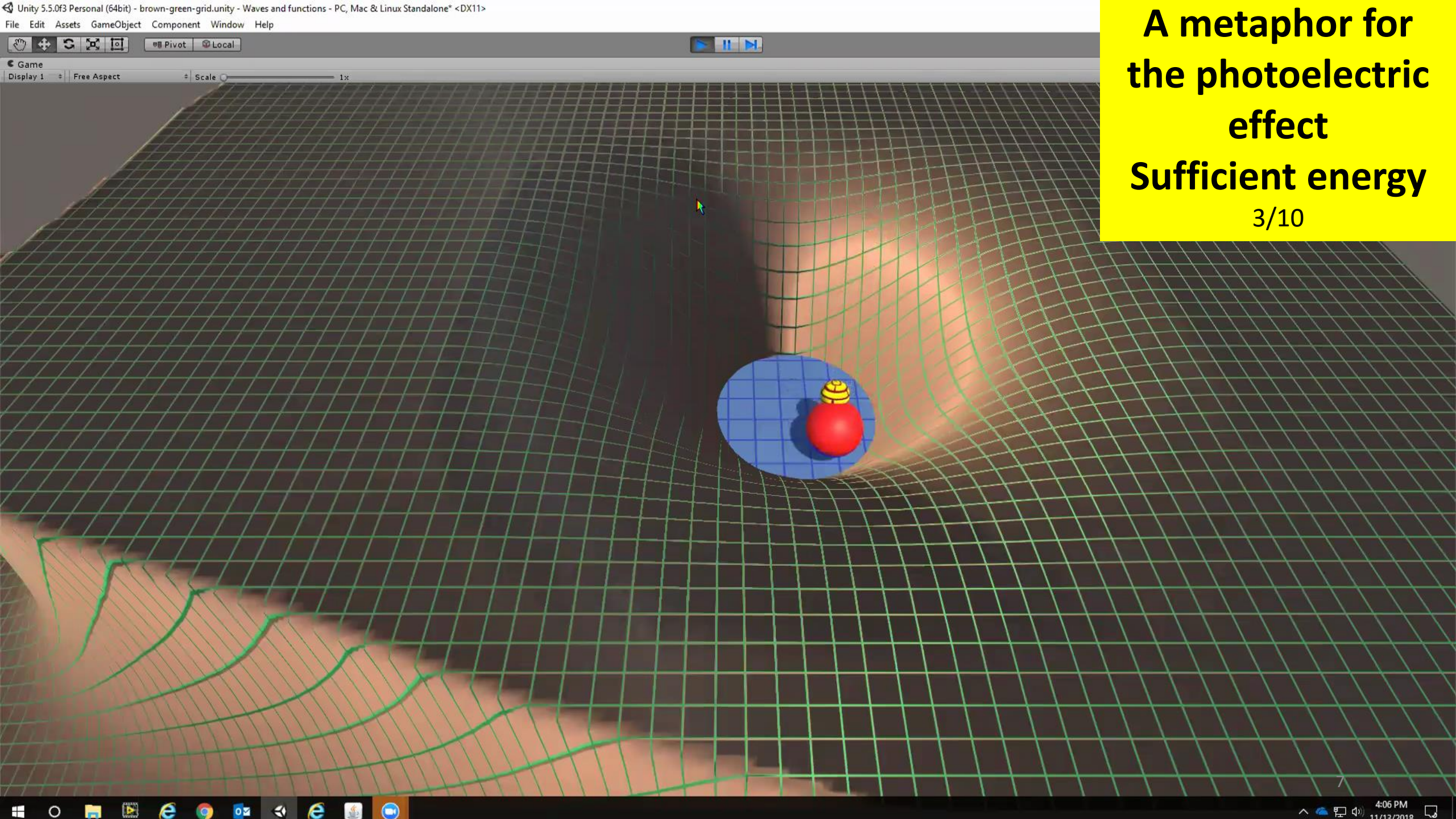
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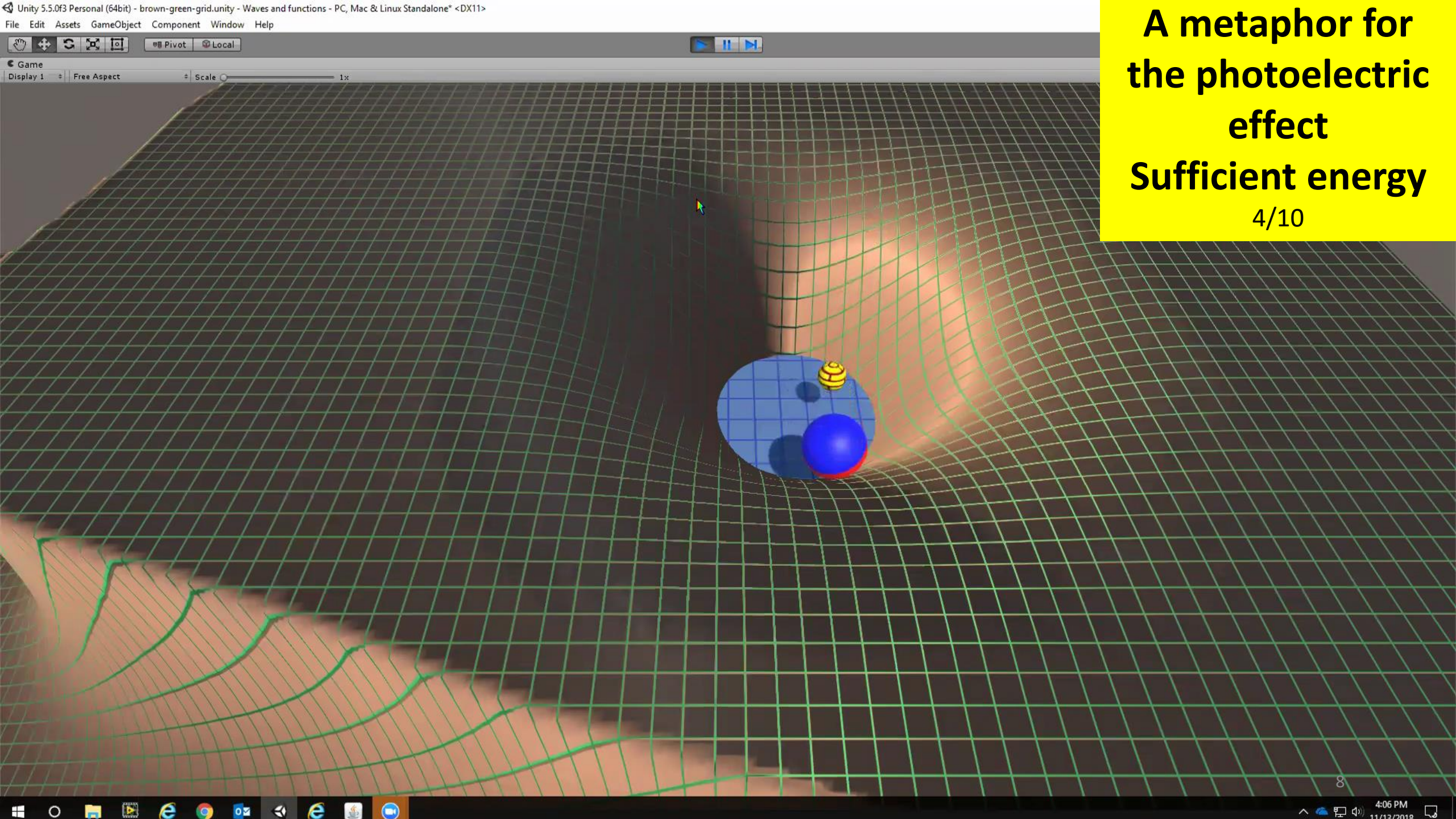
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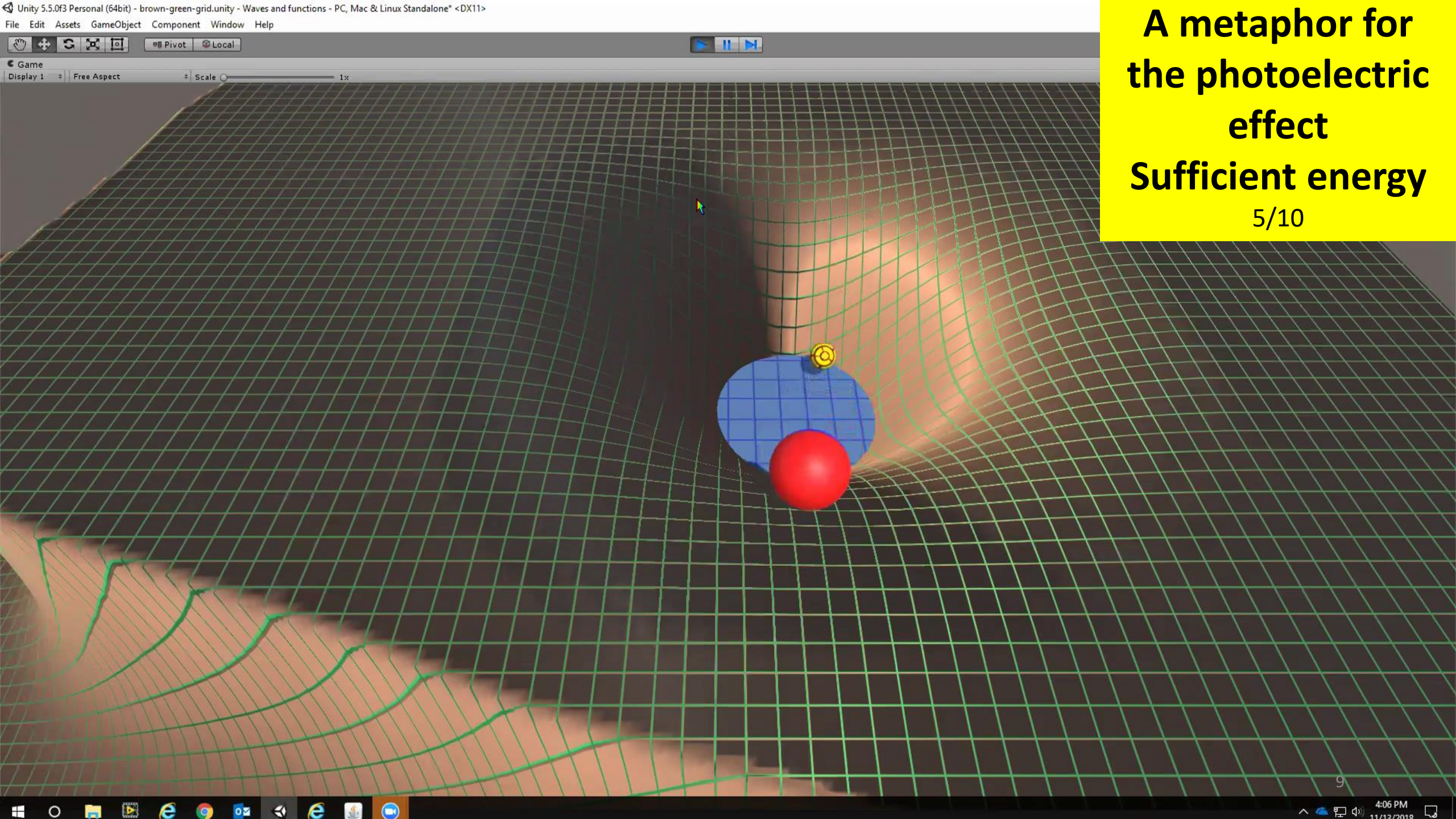
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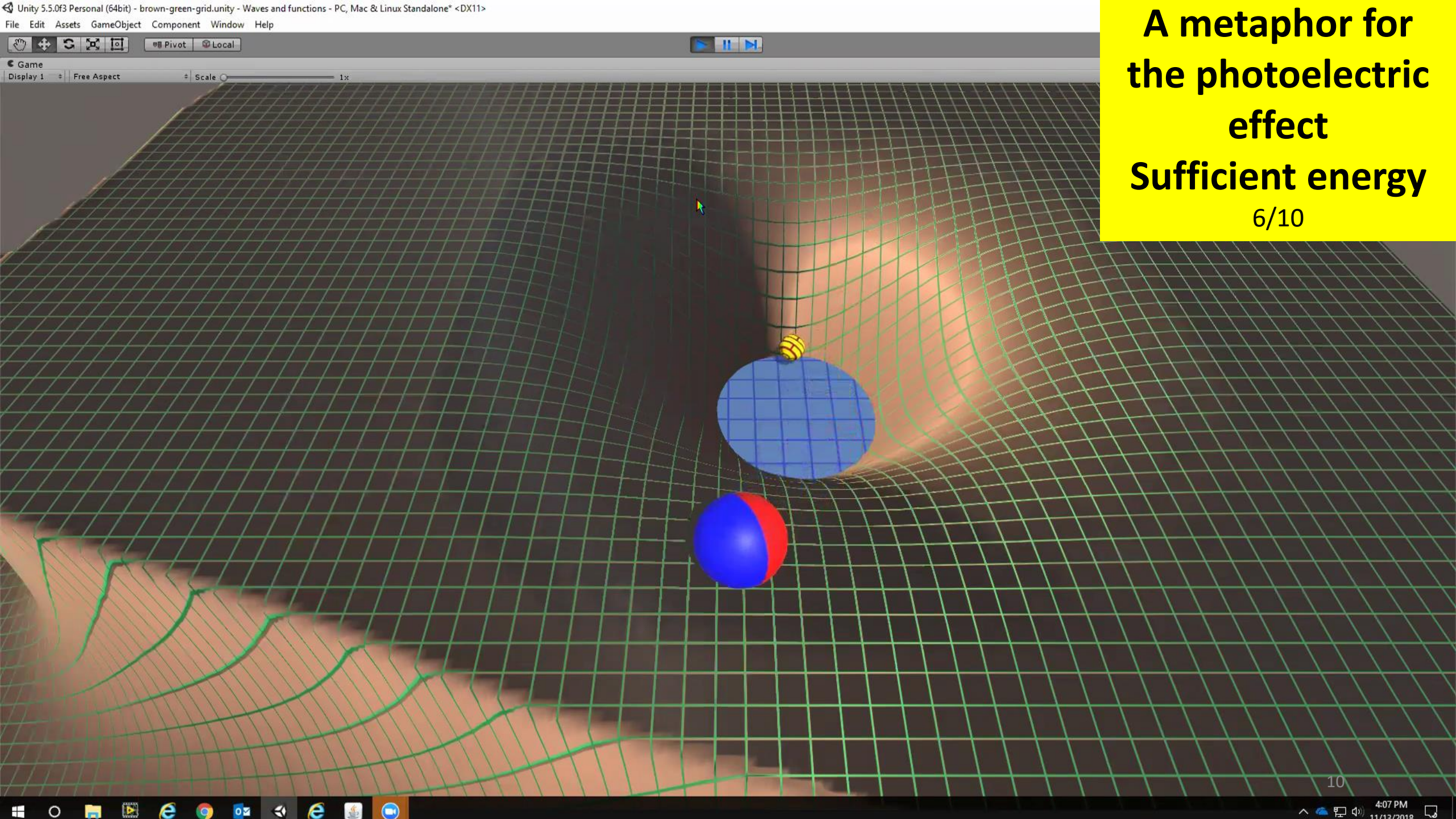
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A metaphor for the photoelectric effect

Sufficient energy

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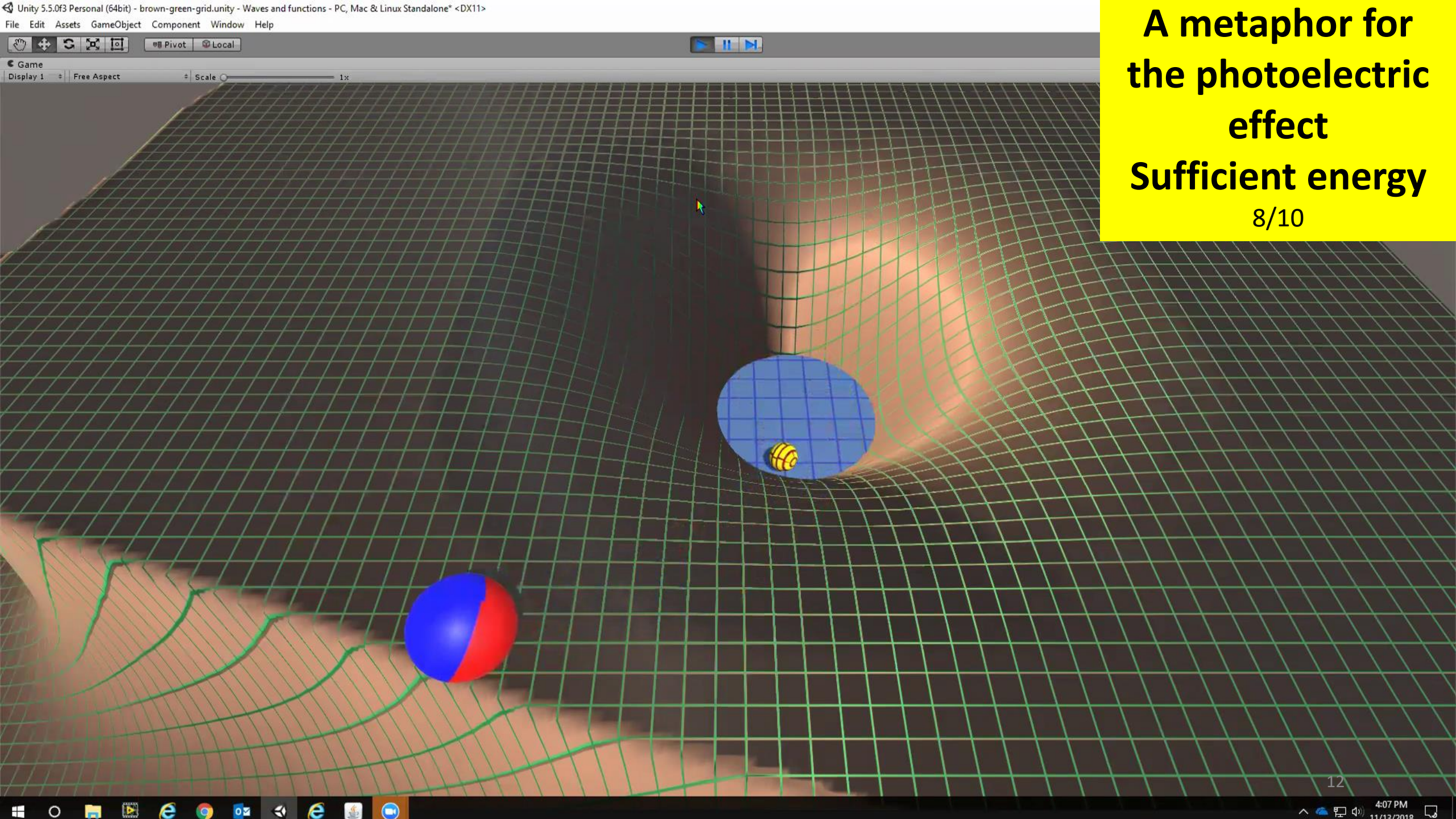
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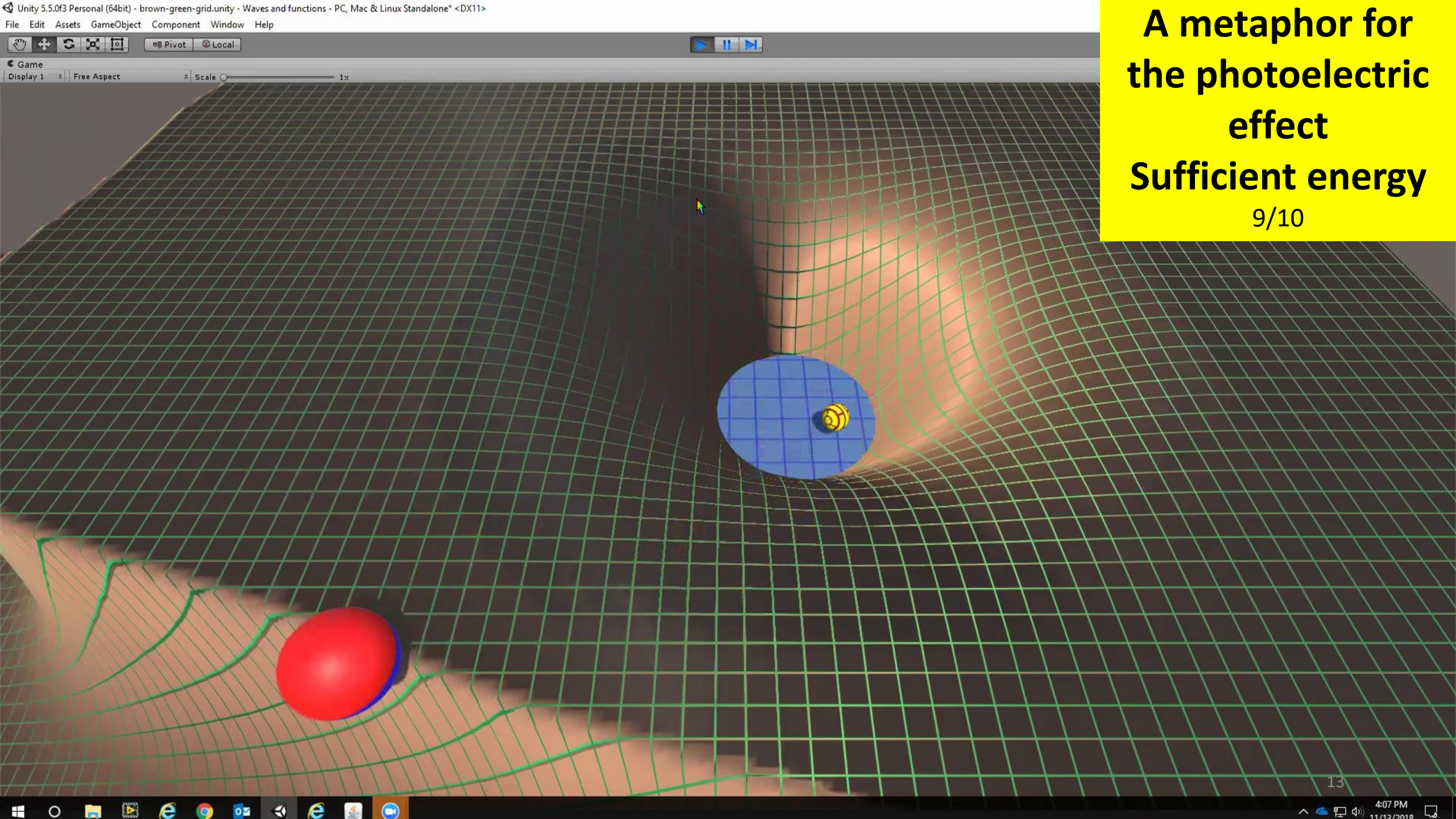
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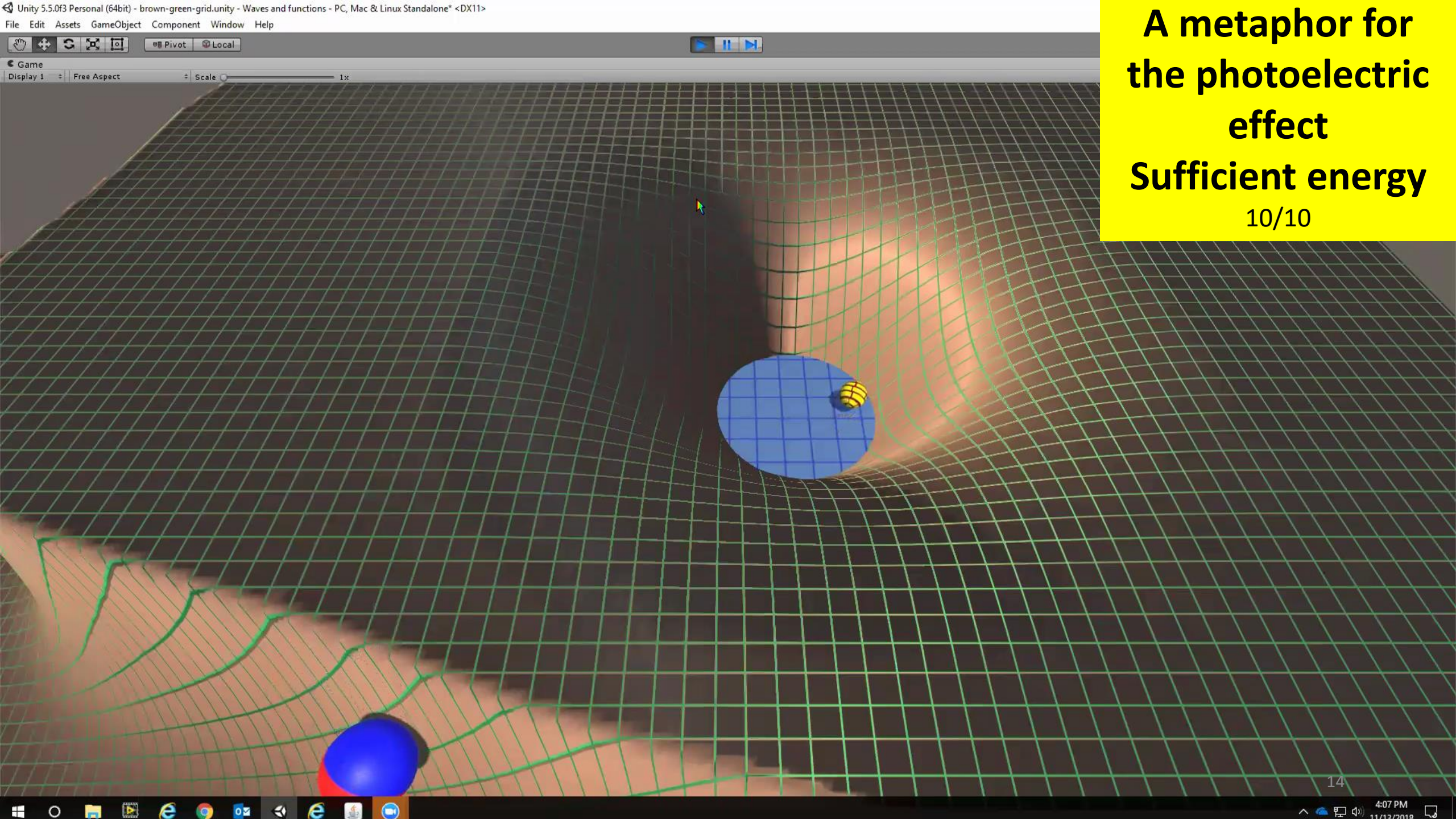
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A metaphor for the photoelectric effect
Sufficient energy
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Photoelectrons can be ejected from metals

- Einstein's Nobel prize was for the explanation of this effect…
- Can compare energy of ejected electrons with original photons to find depth of well…. Useful technique: Photoelectron spectroscopy.

- But what about photons not energetic enough to eject an electron?

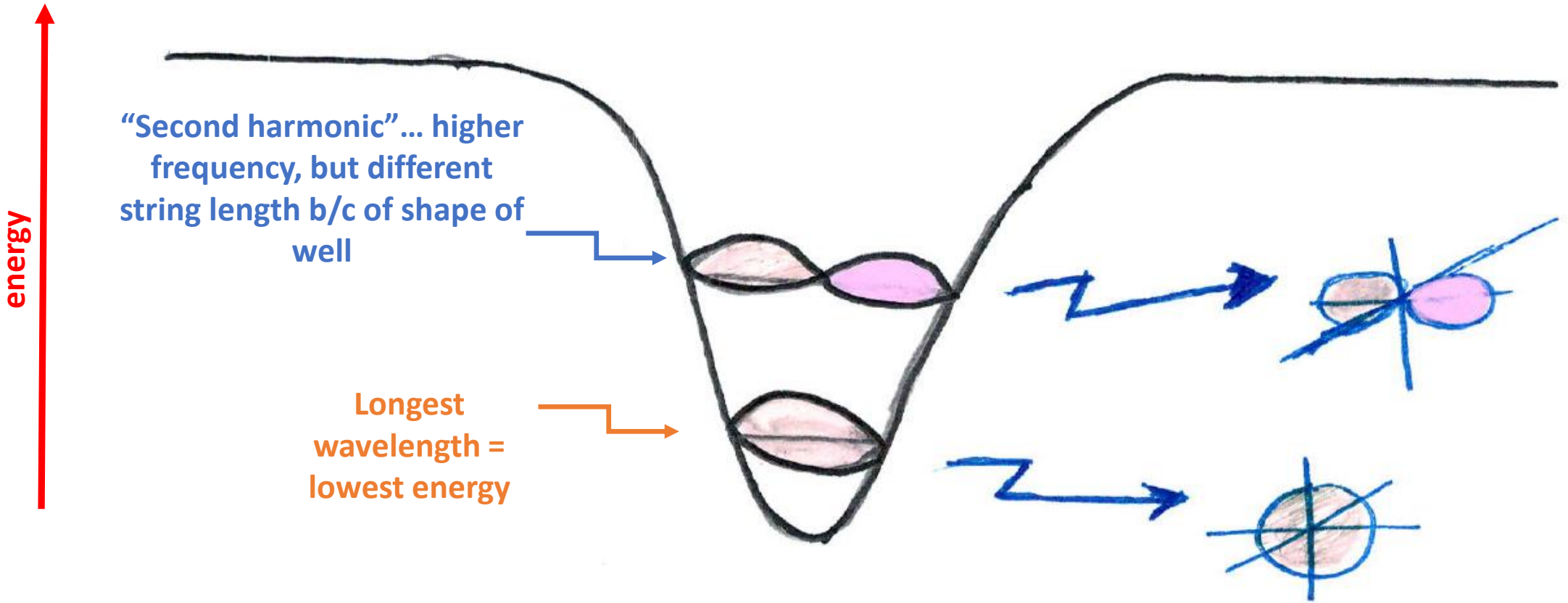
- Energy gets wasted through collisions, heats up the metal, and electron goes back to original situation. ☹

Semiconductors….

- Metals have excellent conductivity… but electrons can move TOO easily.
- Need longer lived charge separation (electron + “hole”) to be able to force electron to return to hole by a route where we can harvest its energy.

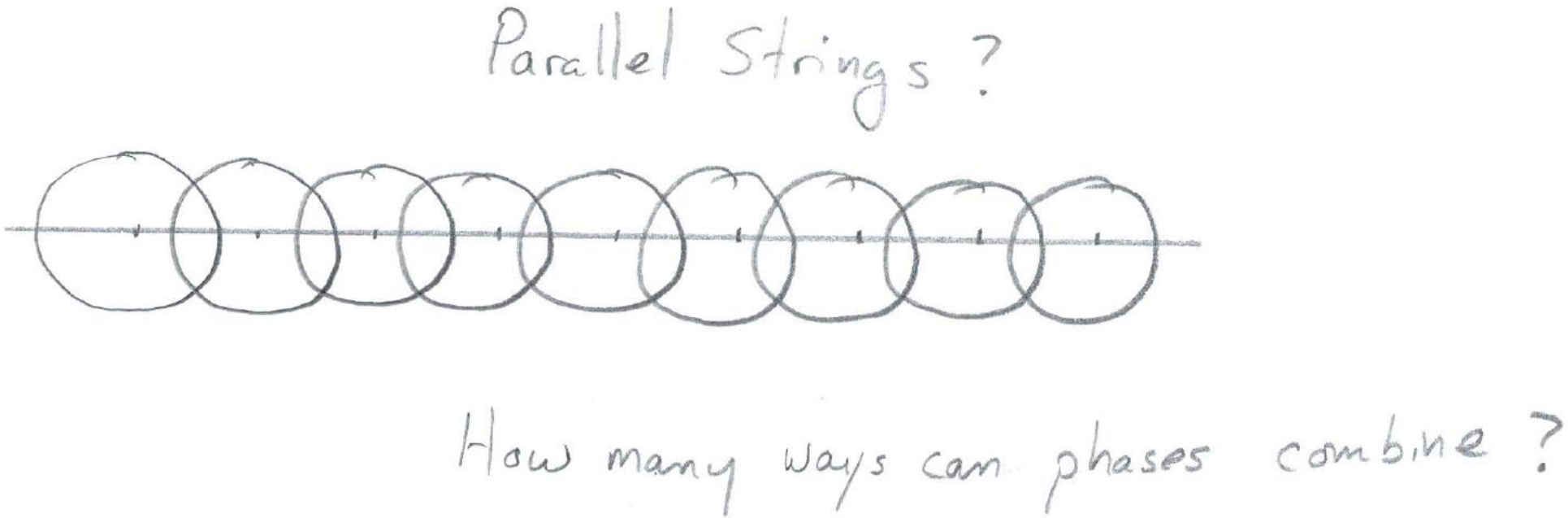
- Semiconductors allow electrons to move, but slowly enough to allow control.
- Perovskites as semiconductors are a recent discovery… but in 10 years, their efficiency in solar cell is as good as 50 years of development on silicon…

Let's talk about how electrons interact with nuclei… Vibrations on a string?



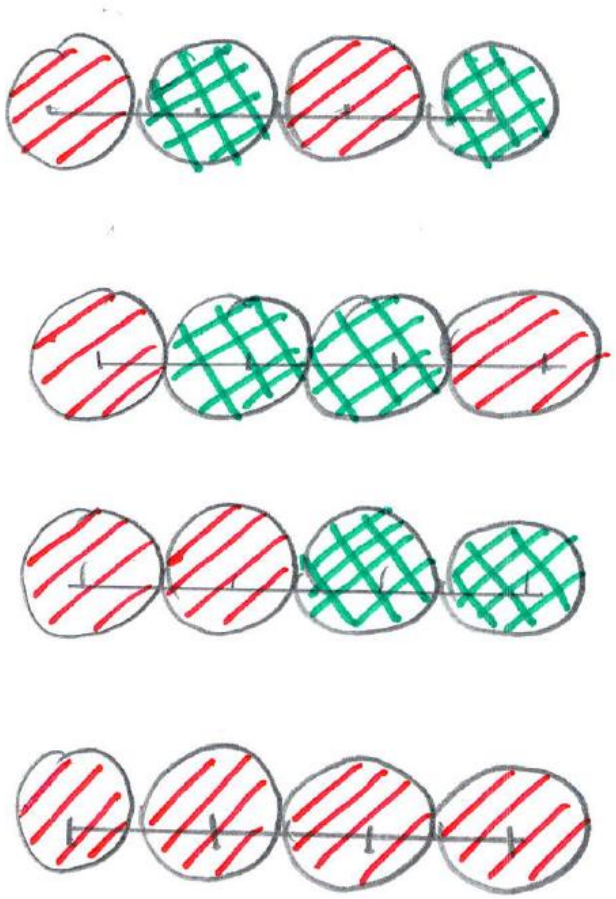
Think of 1-D conductor as a row of atoms

- Electrons on each atom like vibrations on a string…



“Strings” can be in phase or out-of phase…

high energy



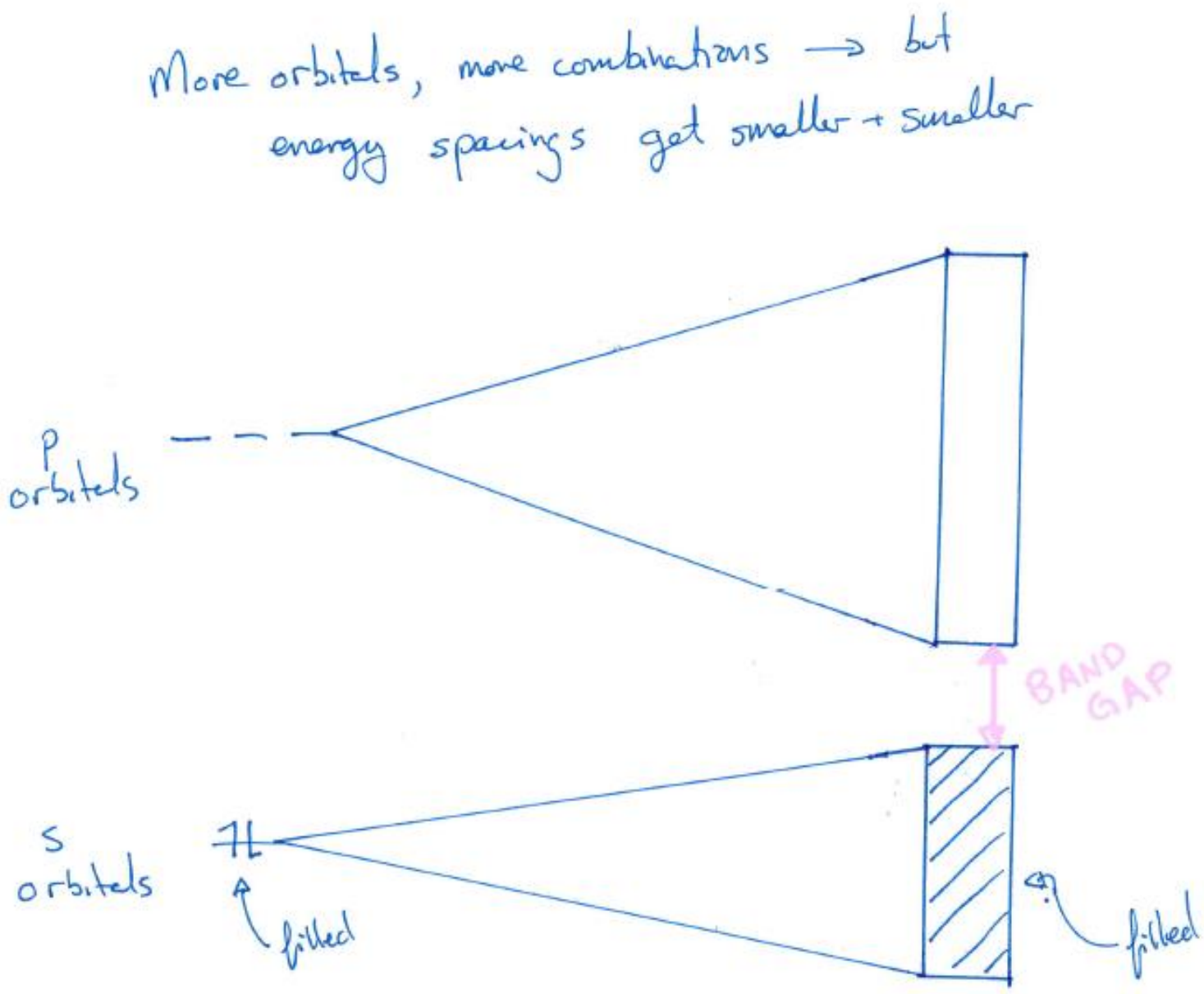
low energy

4 orbitals → 4 ways to arrange phases

End up with an interference pattern which governs where electrons can be.

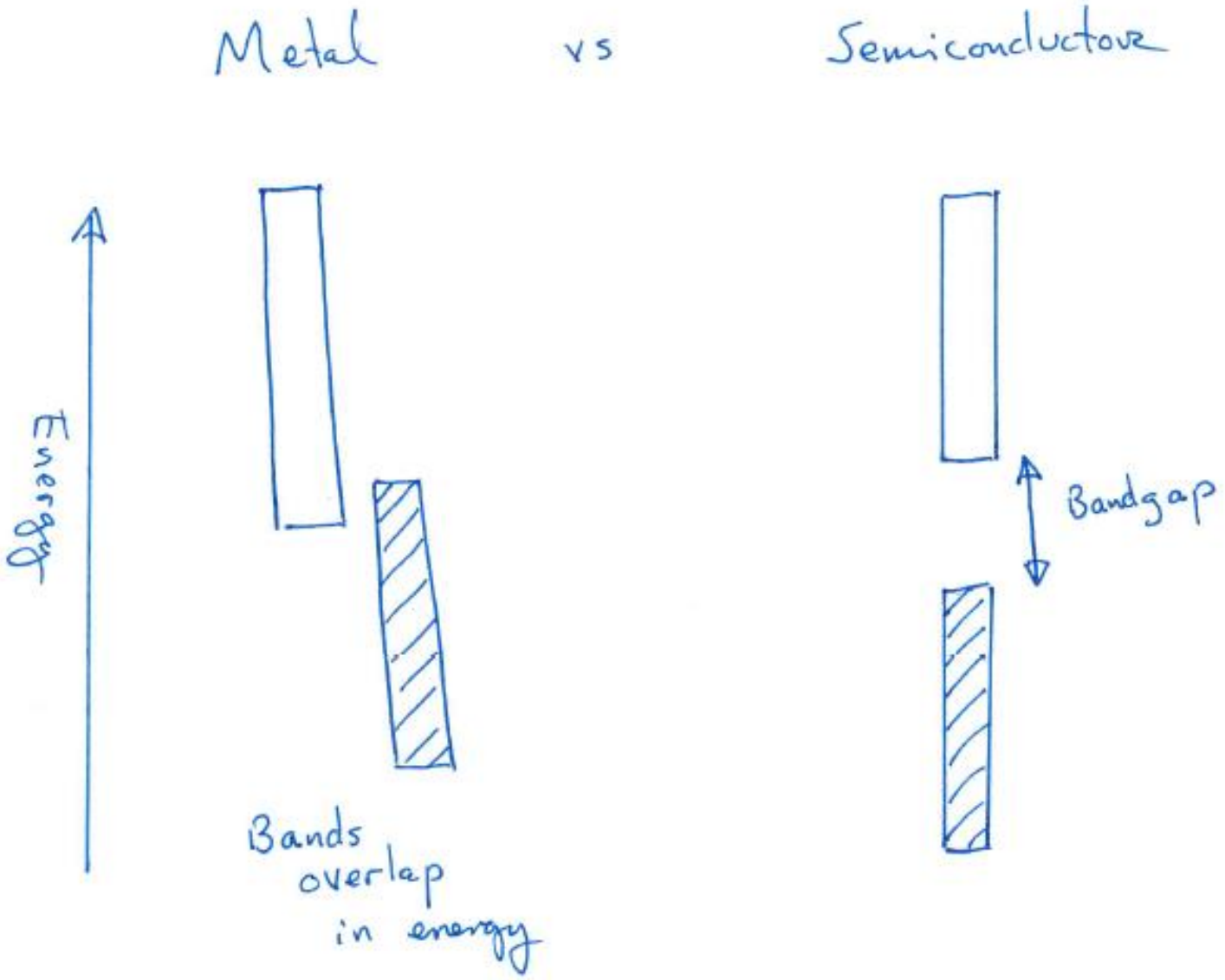
Cartoon of band structure

- Orbitals on neighboring atoms interact by constructive and destructive interference…
- Interference pattern ends up looking like continuous bands with gaps



2 types of conductivity

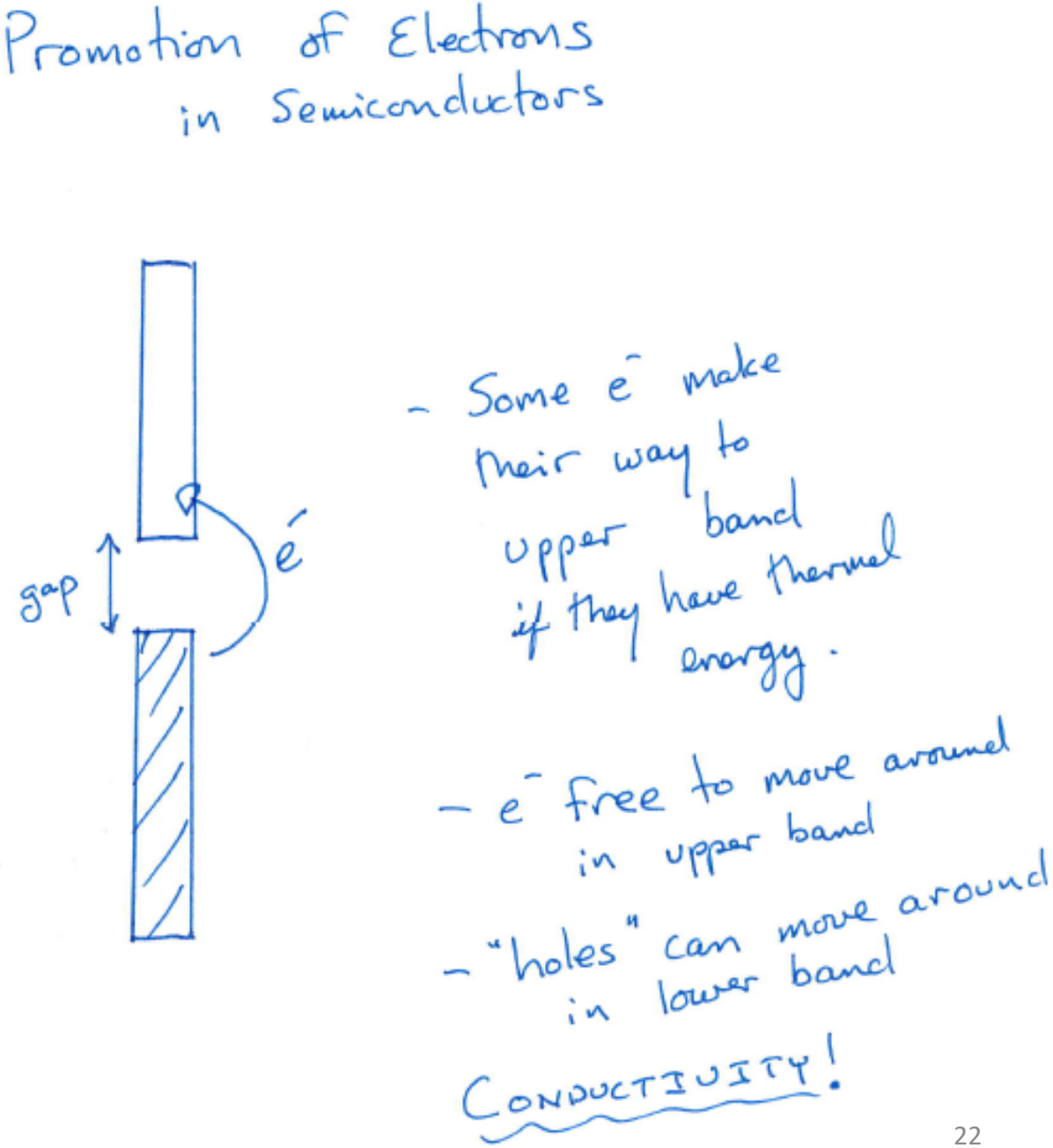
- Orbitals in bands have contributions from whole crystal
- An electron could tunnel to any atom from any atom… delocalization.
- BUT!
- Only if there's some vacant orbitals to move into



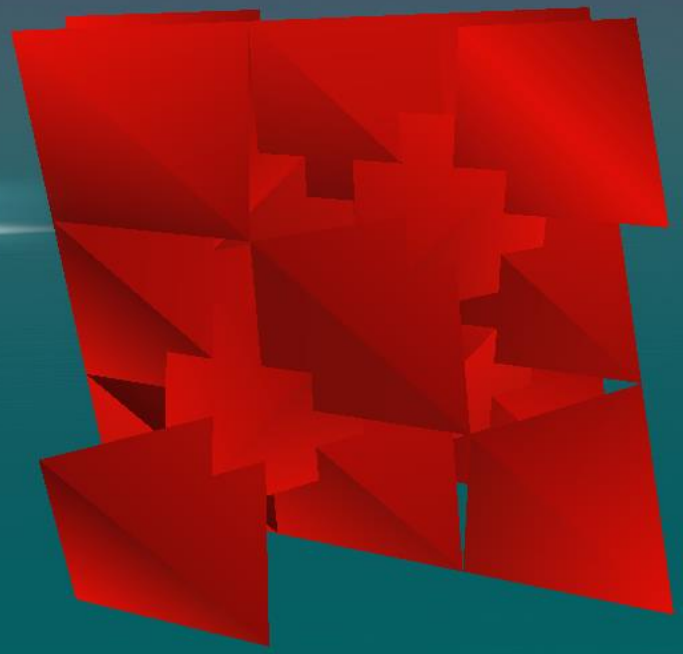
Band Gap!

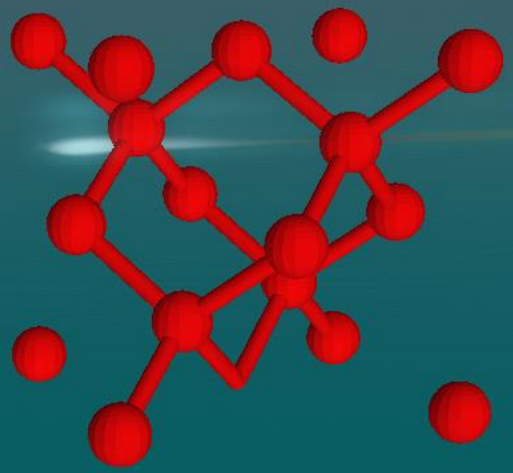
- Semiconductors become more conductive as temperature increases
- More electrons move into upper band

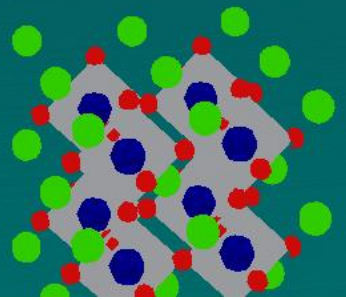
- BTW, technically no such thing as “insulator”… only a semiconductor with HUGE bandgap.



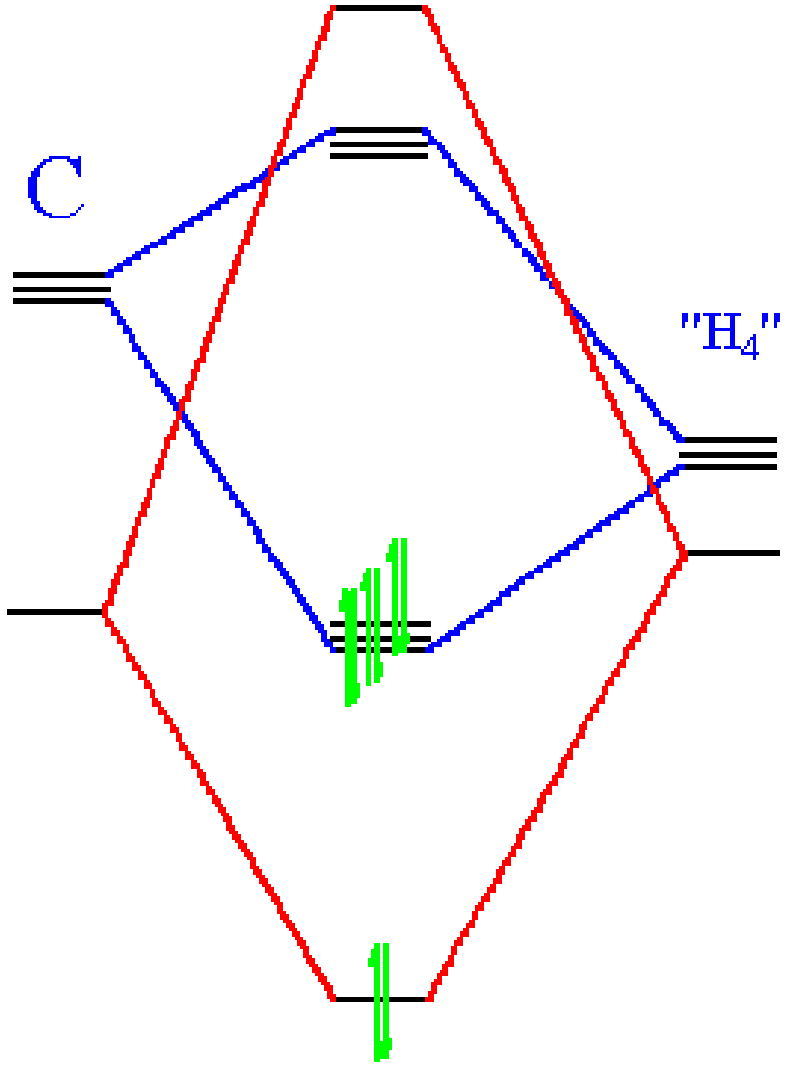
Silicon Structure = Diamond Structure

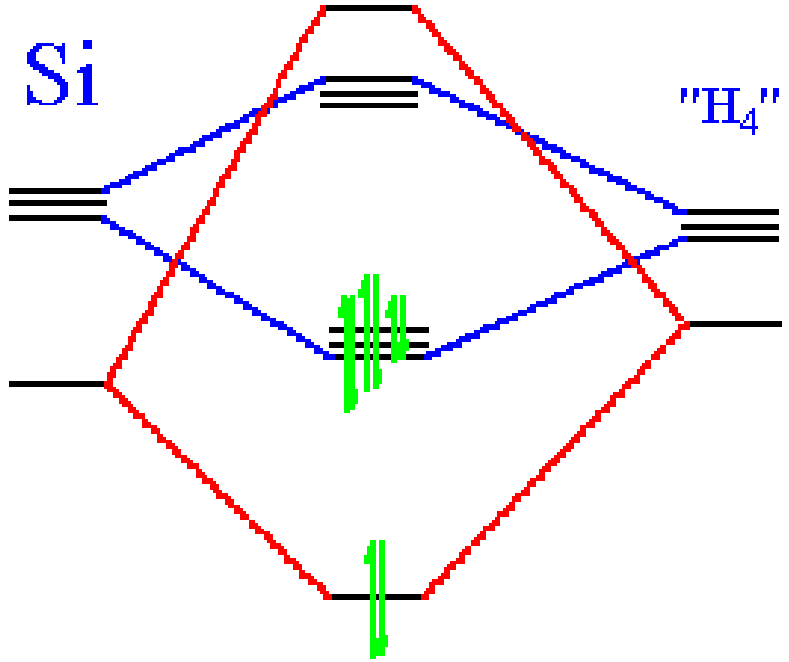






MO's for tetrahedral system



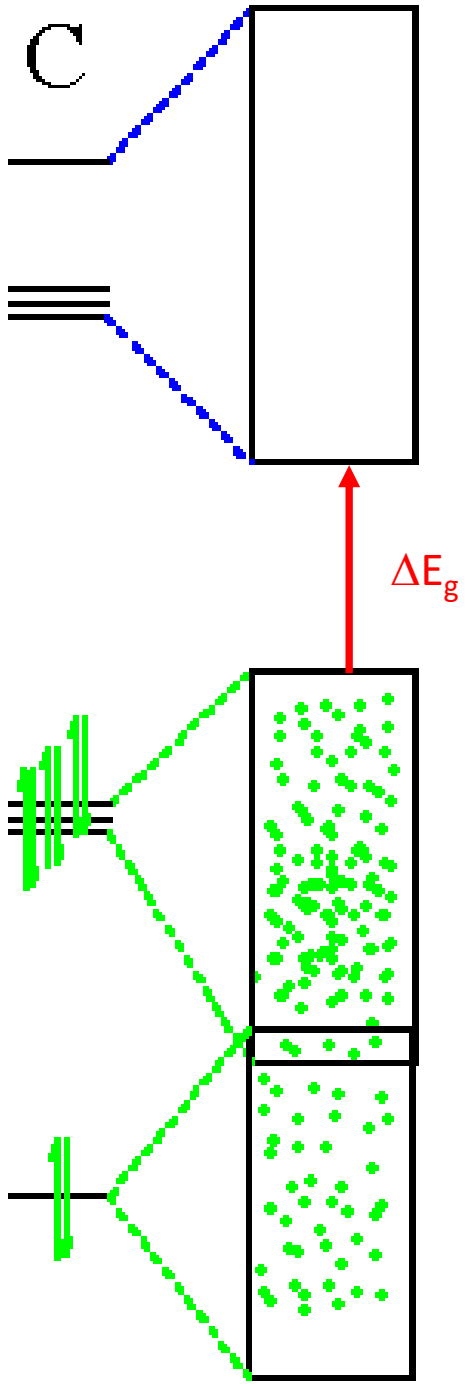


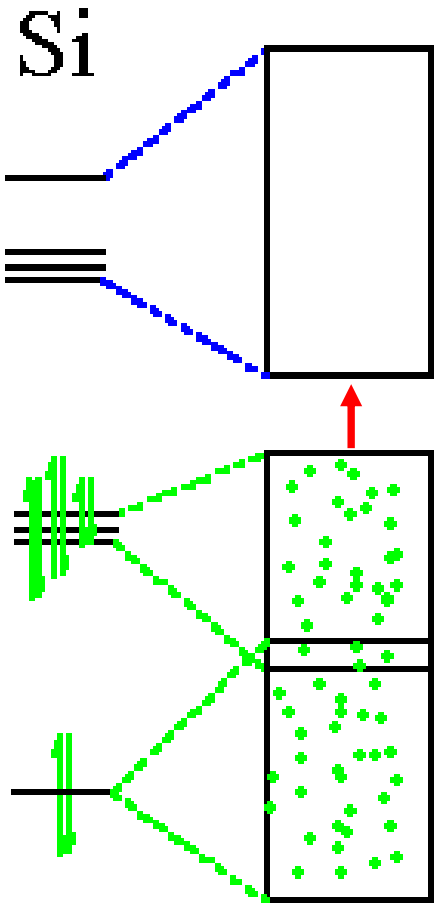
Diamond vs. Silicon

"conduction band"

"band gap, ΔE_g"

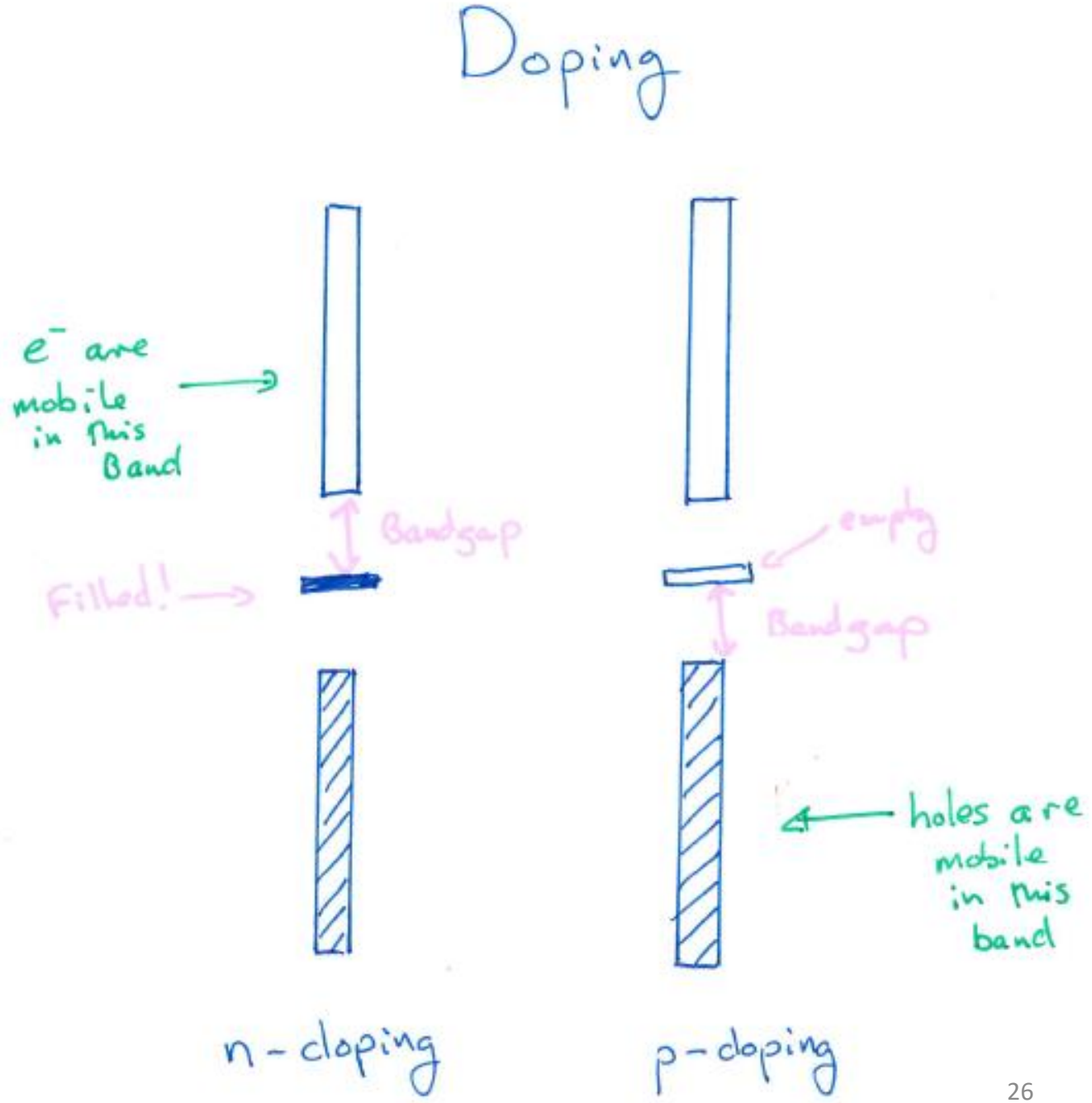
"valence band"





Doping

- Strategy to improve conductivity.
- 1 ppm doping can improve conductivity tremendously
- 0.1% doping can lead to conductivity similar to metals.



p-n junctions

- Also called “diodes”
- If voltage applied so that current flows from left to right, e^- have to lose energy as they jump from n-type to p-type
  - Regular diode, get heat
  - LED, energy comes out as light!
- If no voltage applied, but light absorbed, current will flow right-to-left if it is easier for e^- and holes to migrate outward

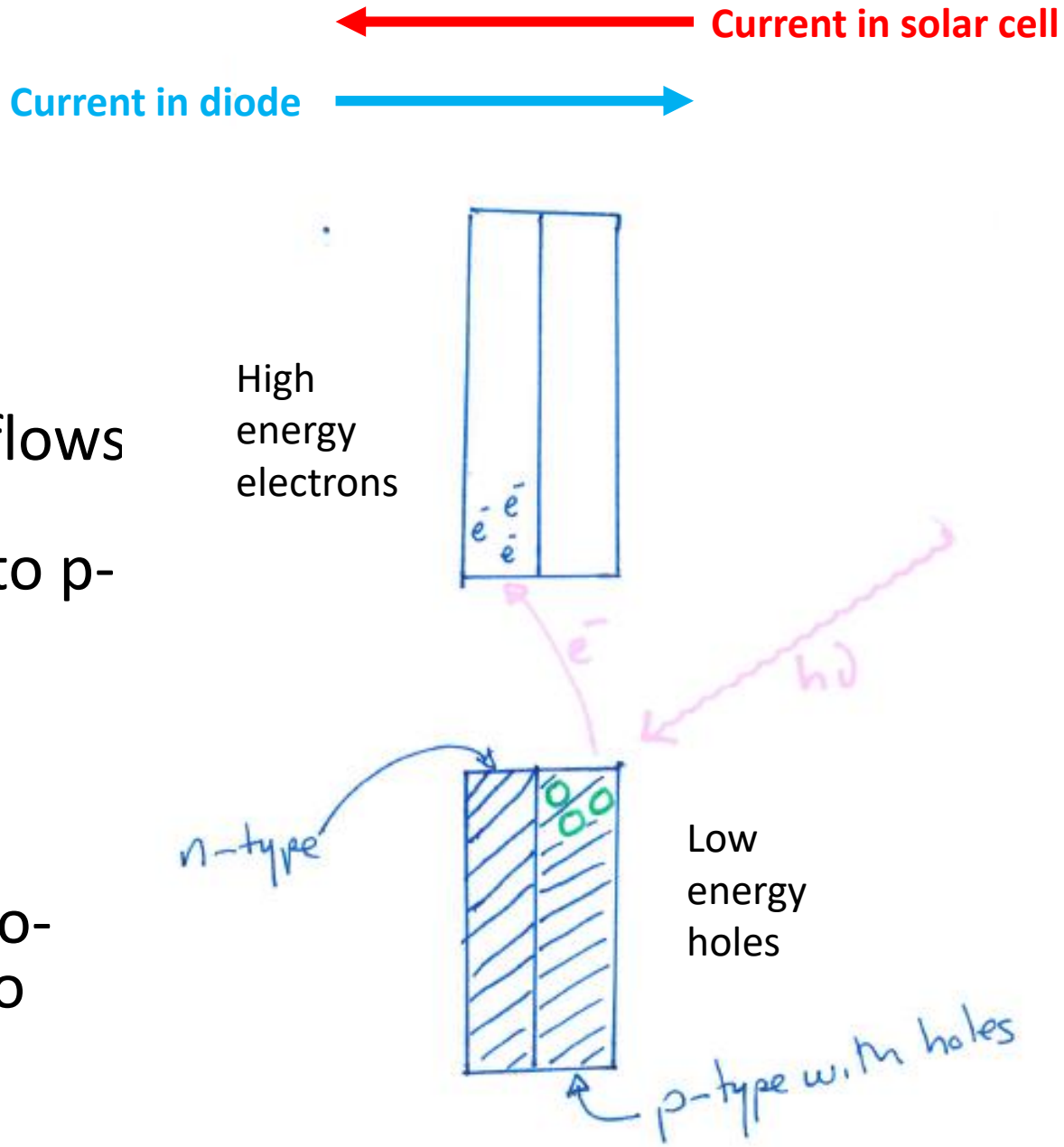
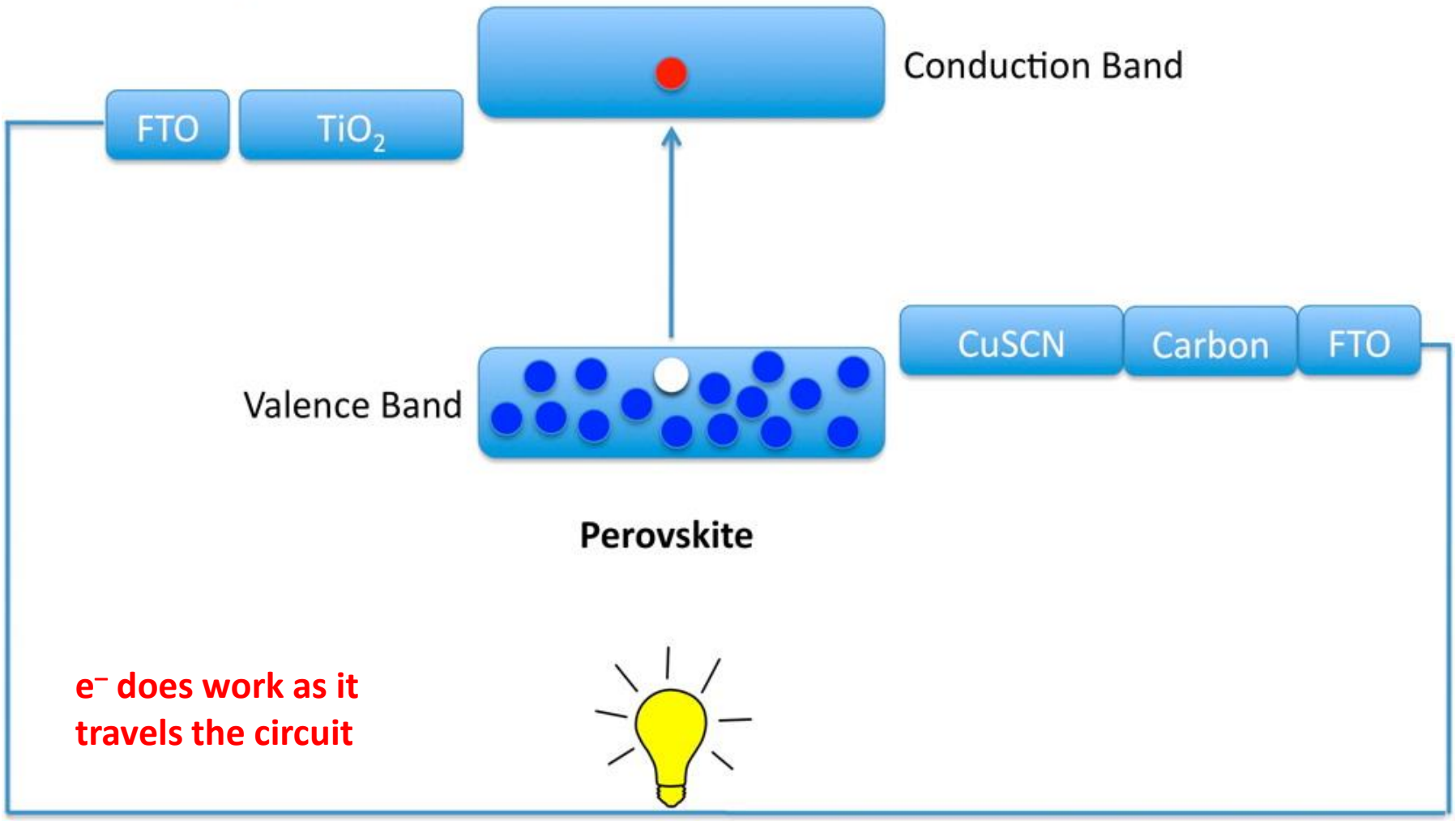


Figure depicting solar cell operation: from light absorption to electrical power generation.



Published in: Sameer Patwardhan; Duyen H. Cao; Shelby Hatch; Omar K. Farha; Joseph T. Hupp; Mercouri G. Kanatzidis; George C. Schatz; *J. Phys. Chem. Lett.* **2015,** 6, 251-255. DOI: 10.1021/jz502648y

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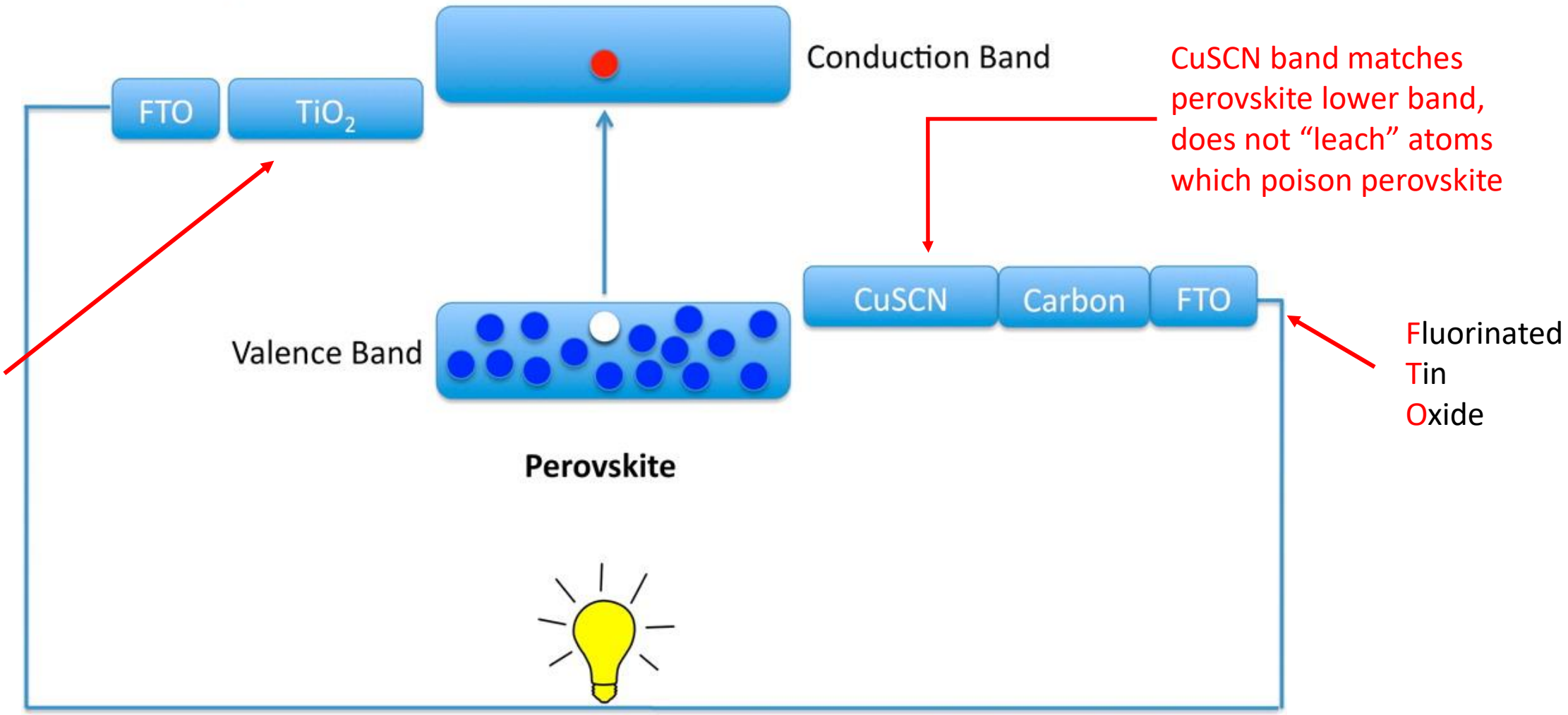

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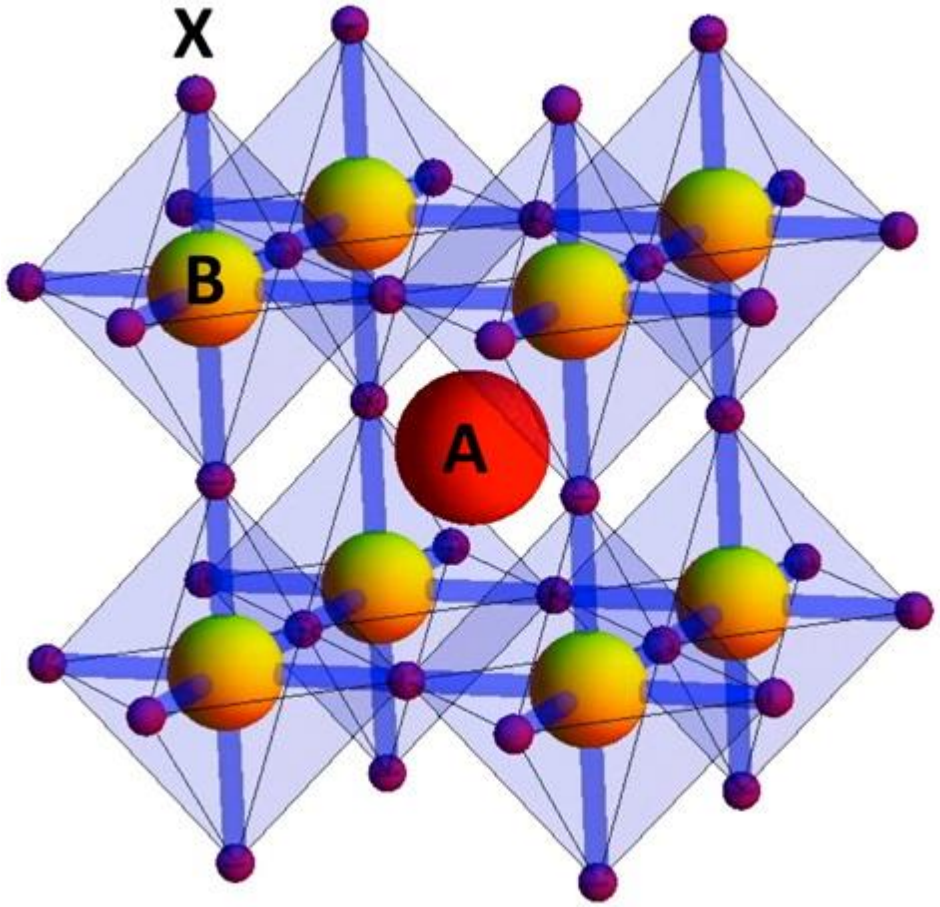
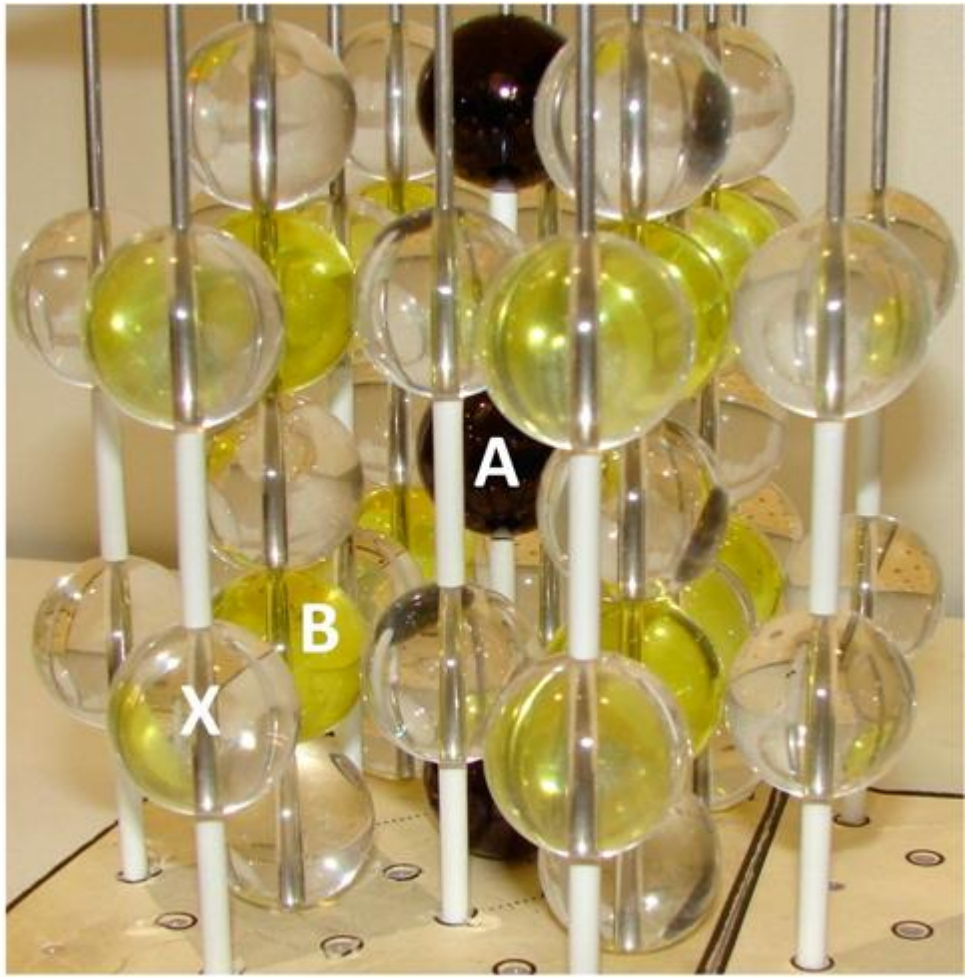
J. Phys. Chem. Lett. **2015,** 6, 251-255. DOI: 10.1021/jz502648y

So what are Perovskites?

- Perovskite is $CaTiO_3$, a common mineral.
- Refers to anything that has a structure similar to $CaTiO_3$
- Often with formula ABX_3
- Each X is connected to 2 B's
- "BX_3" units form an extended lattice with roughly cube-shaped vacant spaces in which "A" sits.

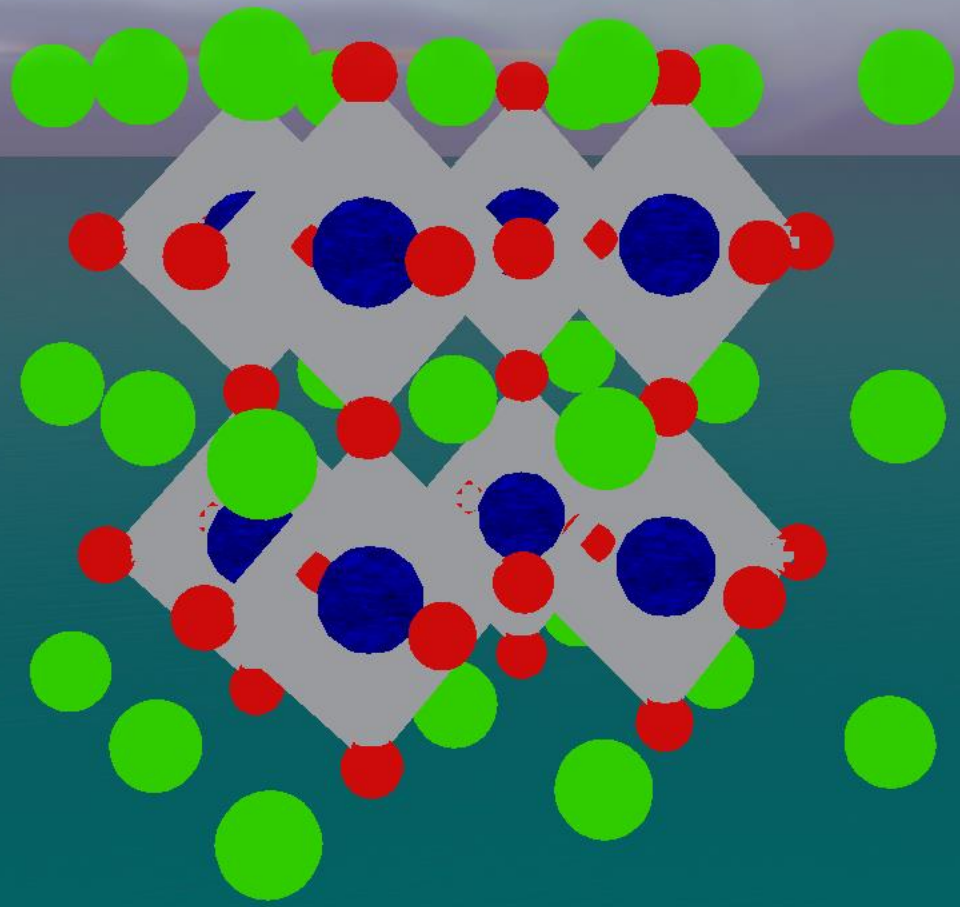




Ideal cubic structure of perovskite, with the general formula ABX_3,
consisting of corner-sharing octahedral (BX_6) with the A-cation occupying a 12-fold coordination site.
The crystal structures were built by a computer program and crystal structure building kit.

Published in: Sameer Patwardhan; Duyen H. Cao; Shelby Hatch; Omar K. Farha; Joseph T. Hupp; Mercouri G. Kanatzidis; George C. Schatz;
J. Phys. Chem. Lett. **2015,** 6, 251-255. DOI: 10.1021/jz502648y

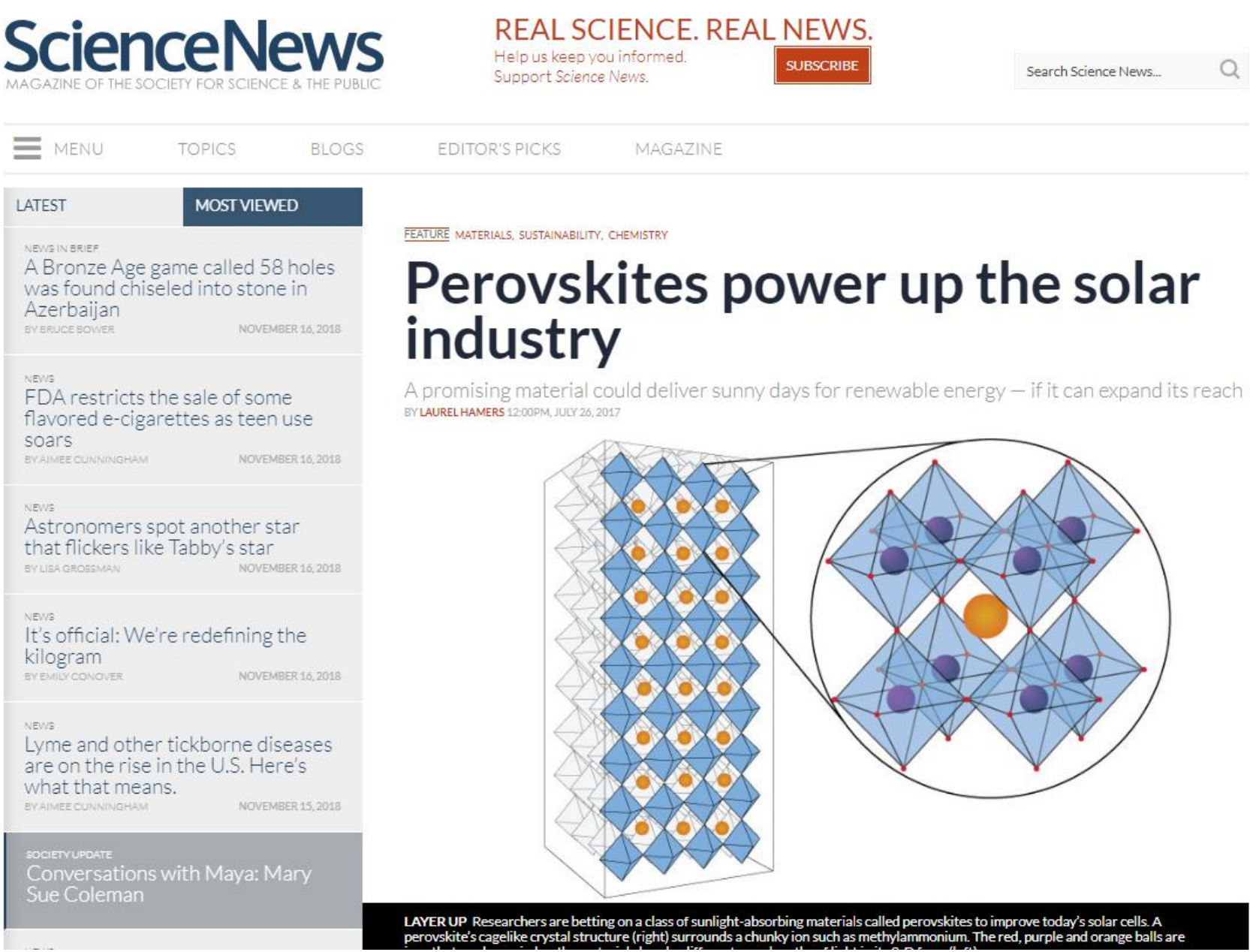
Perovskite: $CaTiO_3$



Similar to Prussian Blue skeleton….

Science News in 2017

- "Perovskite" is a structural motif… like "paisley is a pattern"
- Many materials can exist with this pattern
- A decade of progress with perovskites has resulted in materials as good as > 50 years of silicon solar cell development



https://www.sciencenews.org/article/perovskites-power-solar-industry

Science News often picks up stories later than *C&E News*

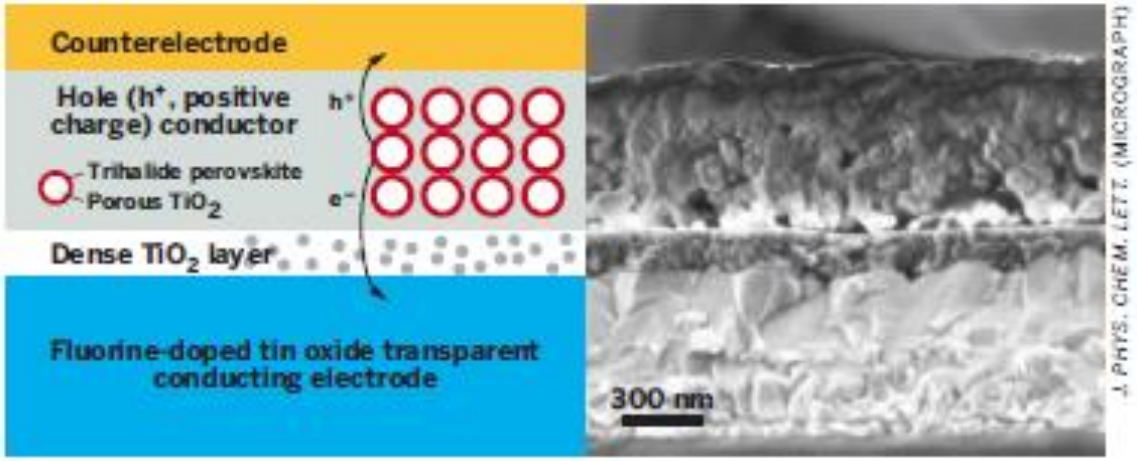
- *Chemical and Engineering News* published by the American Chemical Society weekly.

- I've been following perovskites for a while, since their structure is one of the basic structures taught in undergrad chemistry programs

- It's like finding an exciting new feature on a beloved old device….
  - "You mean my VCR can also control satellites?!?"

As of 2014…

- Feb 2014: 16% efficiency
- Dec 2014: 20.1 % efficiency
- Silicon cells: 25% efficiency



Light passing through a transparent electrode (blue) onto a layer of a photosensitive perovskite material (red) stimulates excitations called electron-hole pairs (e^-/h^+). The charged particles separate and diffuse through the charge-conducting layers to their respective electrodes, thereby generating electric current.

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Perovskite Solar Cells Gain More Ground

MITCH JACOBY

Chem. Eng. News, **2014**, *92* (51), p 21
DOI: 10.1021/cen-09251-cover11
Publication Date: December 22, 2014

openURL

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Cite this: *Chem. Eng. News* 2014, 92, 51, XXX-XXX

RIS Citation GO

Abstract

Tapping the near limitless power of the sun with inexpensive solar cells, many scientists believe, will be necessary to meet future global energy needs. Recent advances in photovoltaic devices featuring light-sensitive materials with the perovskite crystal structure and ABX3 stoichiometry—the most studied example is (CH3NH3)PbI3—are bringing such solar cells closer to reality. Commercial solar cells made with high-purity semiconductors such as silicon convert sunlight to electricity with an efficiency of around 25%, but they are costly. Historically, the efficiency of lower cost cells, such as ones based on polymers or quantum dots, started low and climbed slowly, but only reach around 10% efficiency. In contrast,

Air sensitive? ☹

- This limited the current use of perovskites as solar cells…
- *Nat. Commun.* 2017, DOI: 10.1038/ncomms15218
- Random absences of I^- cause sites where O_2 can be reduced to O_2^-, which then degrades the structure.
- Can be fixed with extra I^- on surface

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Current Issue P

SOLAR ENERGY

Perovskite vulnerability uncovered

Iodide salt coatings protect the promising solar-cell materials from attack by oxygen and light

PDF

Elizabeth Wilson

C&EN, **2017**, *95* (21), pp 6–6 | May 22, 2017

openURL

Cite this: *C&EN* 2017, 95, 21, 6-6

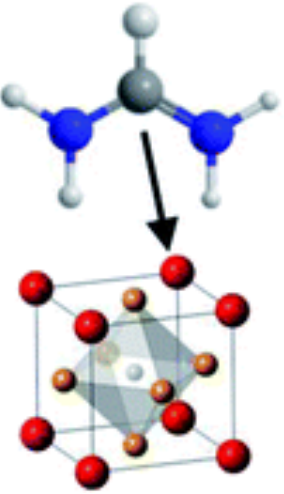
RIS Citation GO

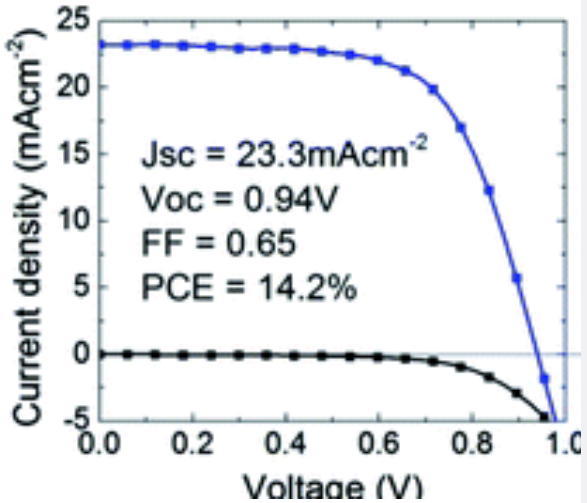
Methylammonium lead halide perovskites ($CH_3NH_3PbI_3$) show great promise for solar-cell materials because they are more efficient at converting sunlight into electricity than current commercial materials are. Perovskite efficiencies can reach 22%, while those of commercial materials are about 15%. However, these perovskites suffer from a serious drawback: They degrade rapidly upon exposure to oxygen and light.

A group including **M. Saiful Islam** at the University of Bath and **Saif A. Haque** of Imperial College London now reports experimental and theoretical evidence for the mechanism behind this degradation (*Nat. Commun.* 2017, DOI: 10.1038/ncomms15218). Their findings have led them to a way to protect these promising materials.

$[FM]PbI_3$

- 2014
- 14.2% efficient,
- But material not as robust





From the journal:
Energy & Environmental Science

Energy Environ. Sci., 2014,**7**, 982-988
DOI: 10.1039/C3EE43822H

Formamidinium lead trihalide: a broadly tunable perovskite for efficient planar heterojunction solar cells

Giles E. Eperon,[a] Samuel D. Stranks,[a] Christopher Menelaou,[a] Michael B. Johnston,[a] Laura M. Herz[a] and Henry J. Snaith*[a]

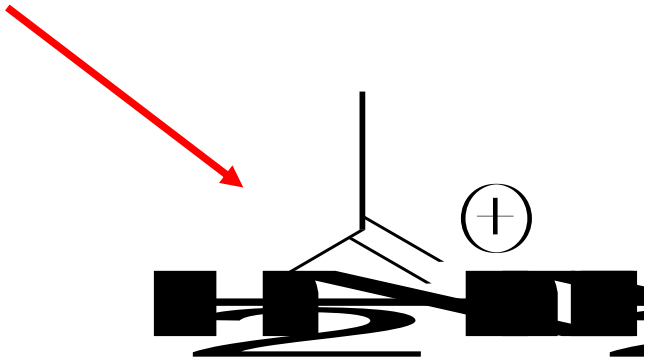
⊕ Author affiliations

Abstract

Perovskite-based solar cells have attracted significant recent interest, with power conversion efficiencies in excess of 15% already superceding a number of established thin-film solar cell technologies. Most work has focused on a methylammonium lead trihalide perovskites, with a bandgaps of ~1.55 eV and greater. Here, we explore the effect of replacing the methylammonium cation in this perovskite, and show that with the slightly larger formamidinium cation, we can synthesise formamidinium lead trihalide perovskites with a bandgap tunable between 1.48 and 2.23 eV. We take the 1.48 eV-bandgap perovskite as most suited for single junction solar cells, and demonstrate long-range electron and hole diffusion lengths in this material, making it suitable for planar heterojunction solar cells. We fabricate such devices, and due to the reduced bandgap we achieve high short-circuit currents of >23 mA cm^{-2}, resulting in power conversion efficiencies of up to 14.2%, the highest efficiency yet for solution processed planar heterojunction perovskite solar cells. Formamidinium lead triiodide is hence promising as a new candidate for this class of solar cell.

As of early 2018…

- 23% efficiency!
- In process of being commercialized!
- Silicon cells: 25% efficiency
- Replace methylammonium (MA) by foramidinium, Rb^+ and Cs^+



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Current Issue

SOLAR POWER

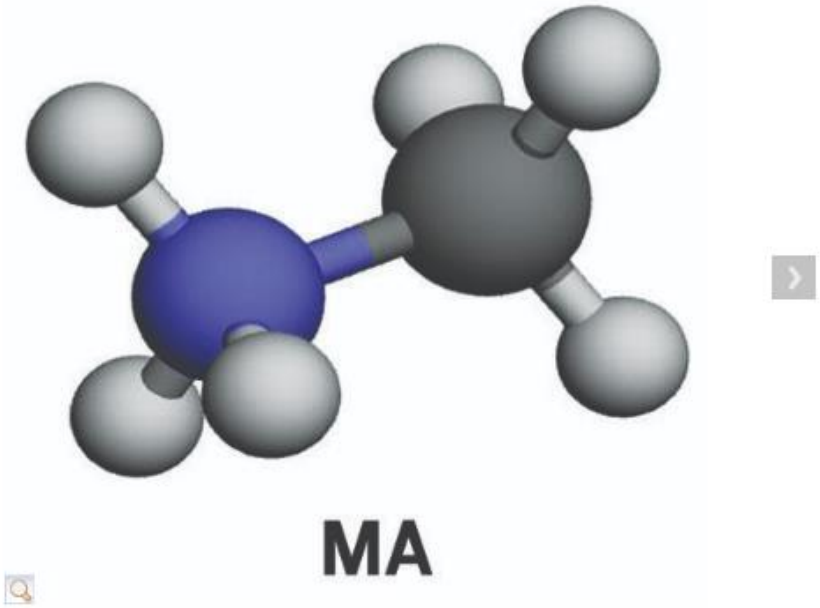
Stabilizing perovskite solar cells

Replacing commonly used methylammonium component with formamidinium group and metal ions leads to long lasting device

Mitch Jacoby
C&EN, **2018**, *96* (41), pp 10–10 | October 15, 2018

Cite this: *C&EN* 2018, 96, 41, 10-10

RIS Citation GO



Replacing commonly used methylammonium (MA) compounds with ones based on formamidinium (FA) can boost perovskite solar cell stability. (Credit: Michael Saliba)

Commercial Development

- Company is *Oxford PV* in UK
- Test unit at 25.2%
- 243 cm^2 modules from assembly line at 24% (shown at left)
- Run for “thousands of hours at 60°C”
- Withstand -40°C to 85°C
- Withstand 85% humidity at 85°C

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Subs

Current Issue Pa

SOLAR POWER

Perovskite progress pushes tandem solar cells closer to market

Rapid improvements in the stability and efficiency of perovskite-silicon tandem cells are raising commercial hopes

Mark Peplow, special to C&EN

C&EN, **2018**, *96* (24), pp 16–18 | June 11, 2018

openURL

Cite this: *C&EN* 2018, 96, 24, 16-18

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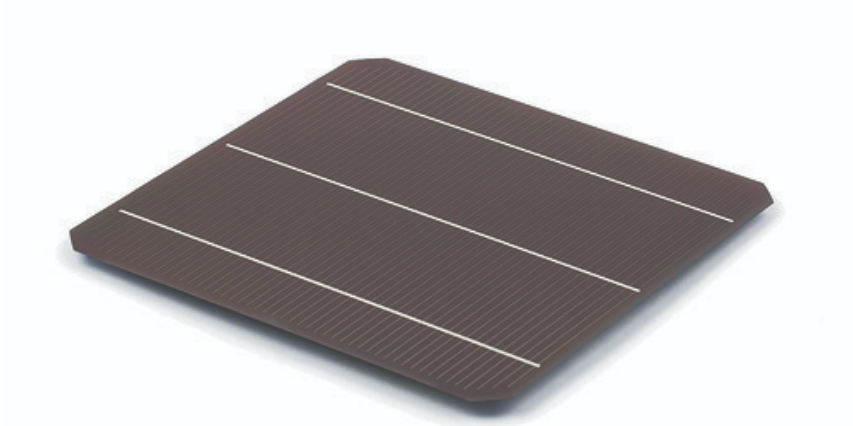
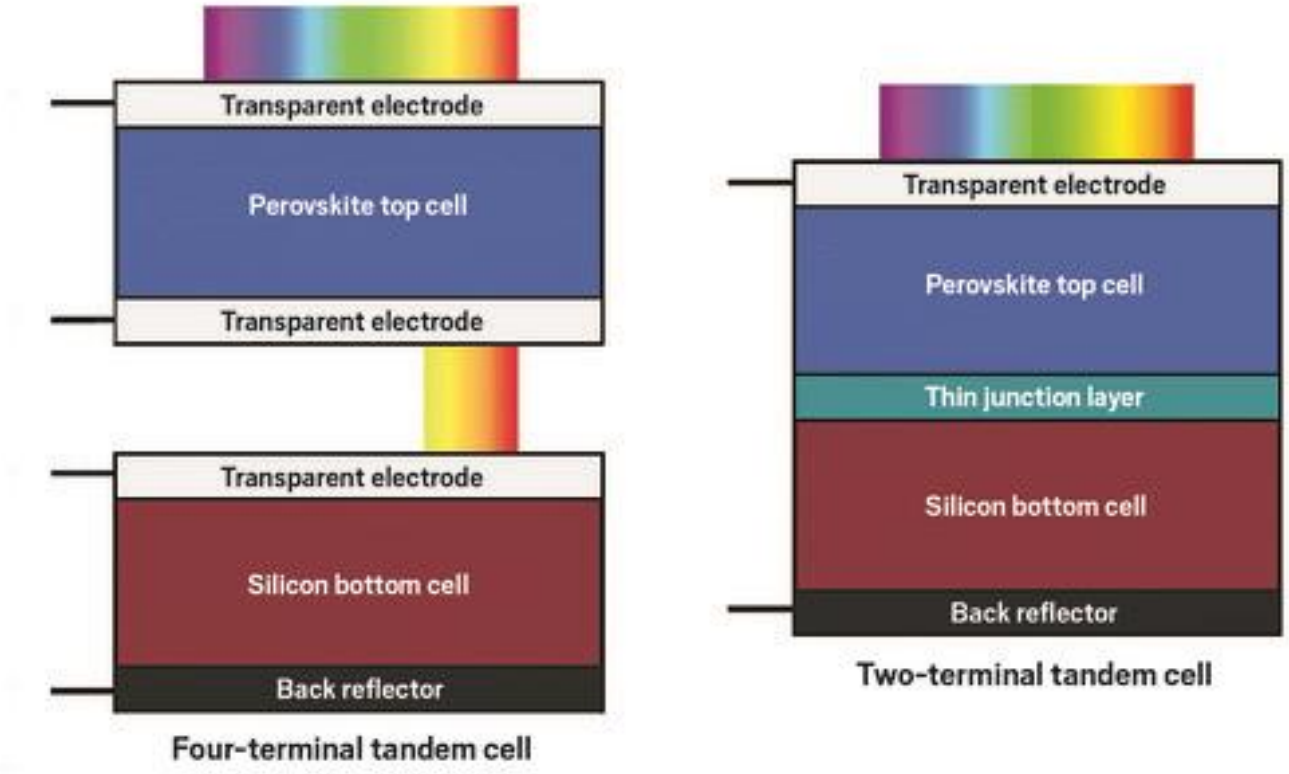


Oxford PV's designs

- Easier to fabricate than Si cells, leading to a lower CO_2 footprint and overall low toxicity footprint, despite containing Pb.

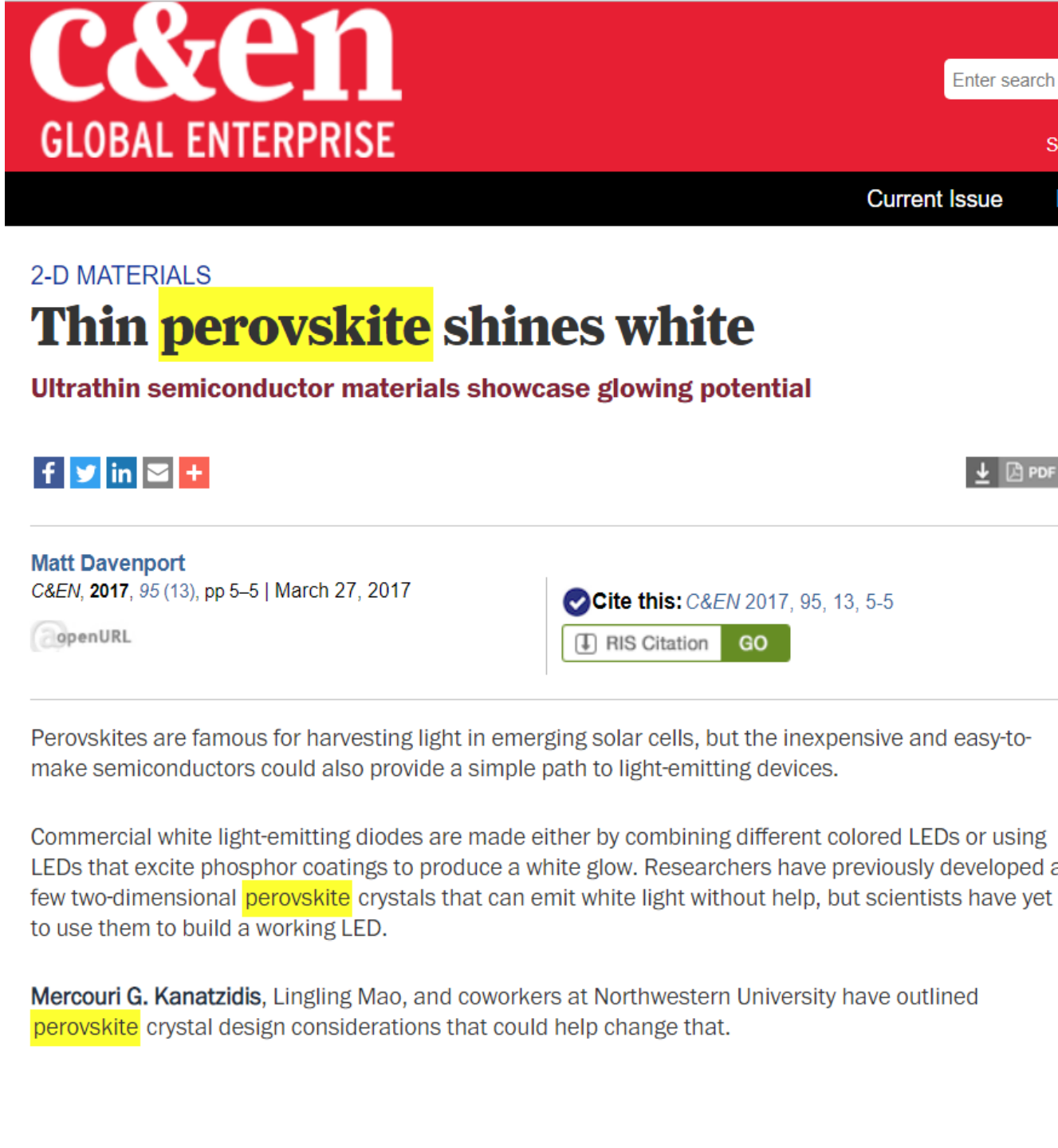
- Looks like first commercial facility to manufacture these cells will be operational in 2020.



Researchers can build tandem solar cells by simply placing one cell on top of another (left) or integrating the materials into a single stack (right). (Credit: Adapted from Adv. Mater. Interfaces)

LED's?

- With the right materials, an LED is simply a solar cell running in reverse
- Apply voltage to cell to force e^- to move…
- If lucky, emit photons as e^- jump down from conduction band in n-type semiconductor to conduction band in p-type semiconductor.



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Current Issue

2-D MATERIALS

Thin perovskite shines white

Ultrathin semiconductor materials showcase glowing potential

Matt Davenport

C&EN, **2017**, *95* (13), pp 5–5 | March 27, 2017

openURL

Cite this: *C&EN* 2017, 95, 13, 5-5

RIS Citation GO

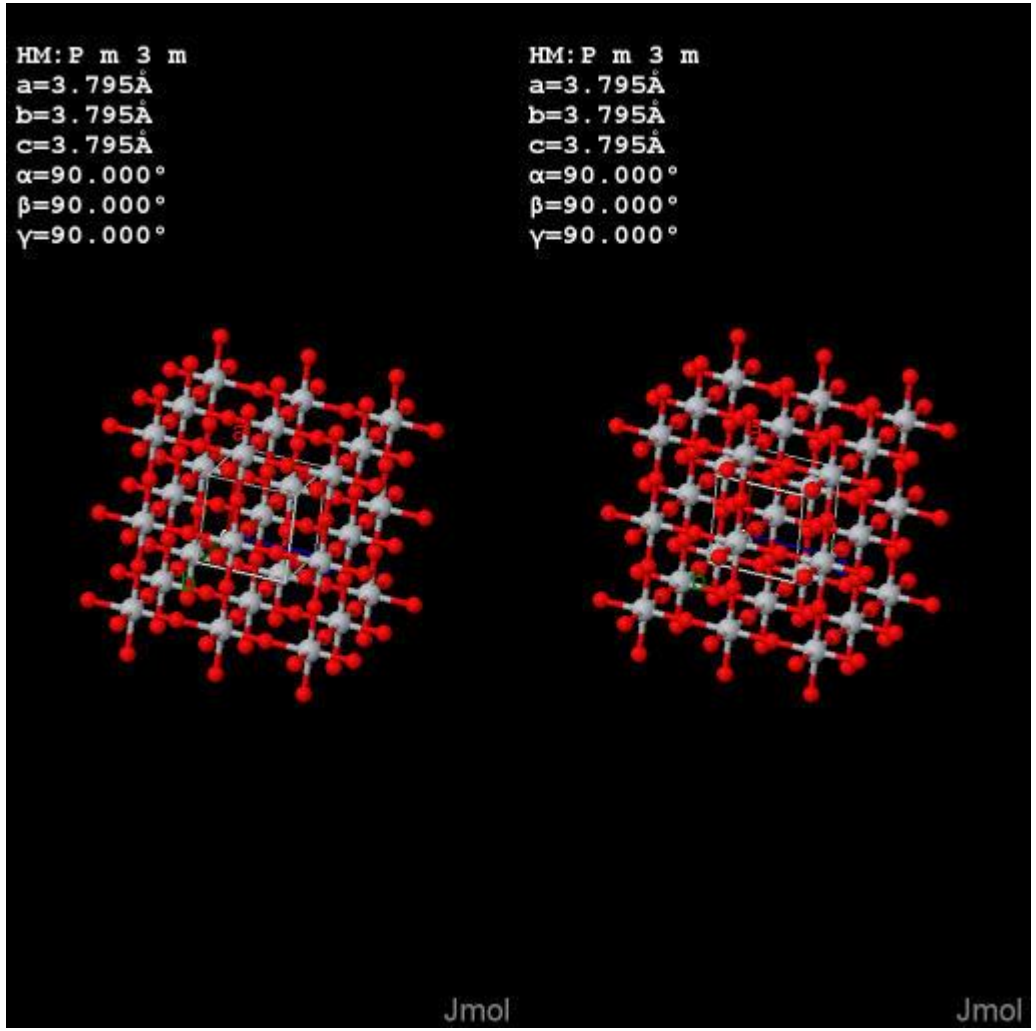
Perovskites are famous for harvesting light in emerging solar cells, but the inexpensive and easy-to-make semiconductors could also provide a simple path to light-emitting devices.

Commercial white light-emitting diodes are made either by combining different colored LEDs or using LEDs that excite phosphor coatings to produce a white glow. Researchers have previously developed a few two-dimensional perovskite crystals that can emit white light without help, but scientists have yet to use them to build a working LED.

Mercouri G. Kanatzidis, Lingling Mao, and coworkers at Northwestern University have outlined perovskite crystal design considerations that could help change that.

Wall-eyed stereogram

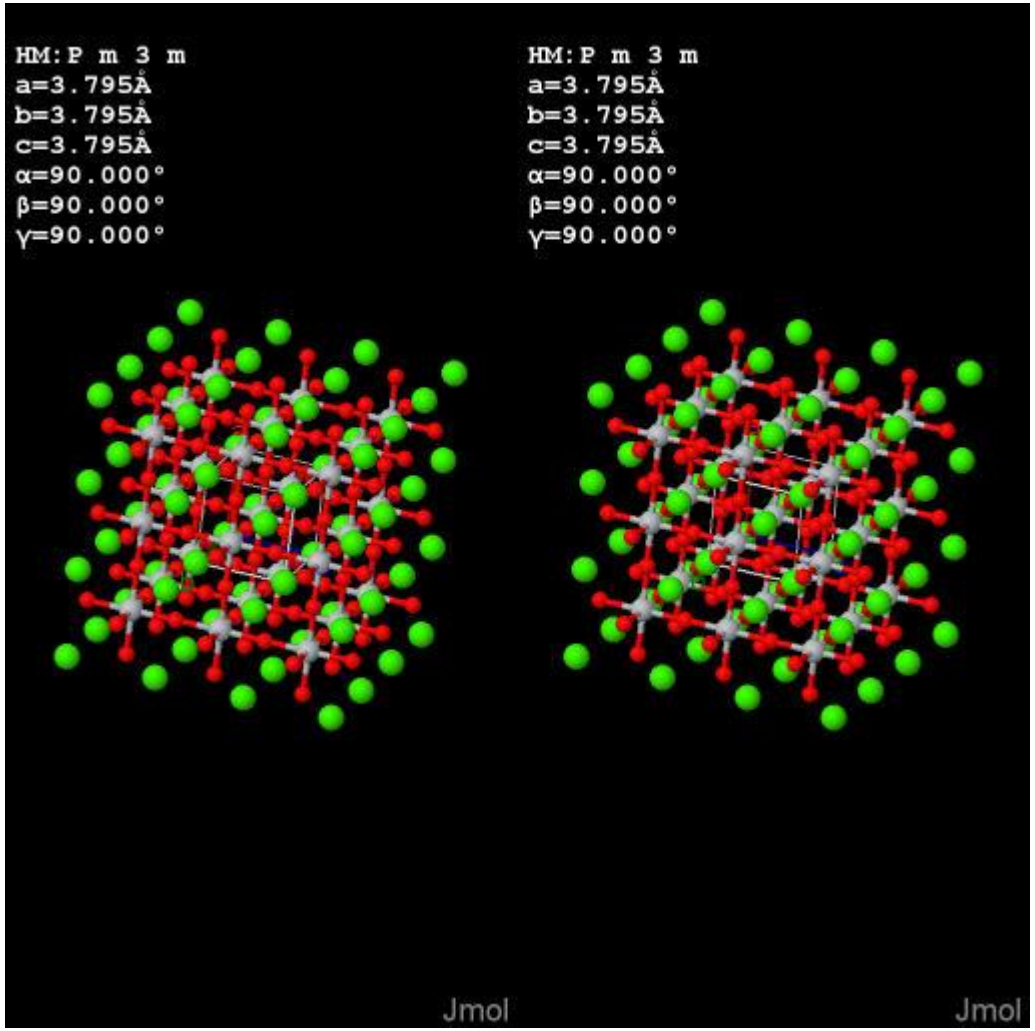
- “Magic eye view”… reading glasses are helpful
- Need to be 10-15 cm from screen, with image flat relative to your face, right in front of screen
- This view just shows the Ti atoms linked together along all x, y, and z axes by red O-atoms
- Ca atoms not shown



Barth, T. “Perovskite,” *Norsk Geologisk Tidsskrift* **1925**, *8*, 201-216.
http://rruff.geo.arizona.edu/AMS/download.php?id=18905.amc&down=amc

Wall-eyed stereogram

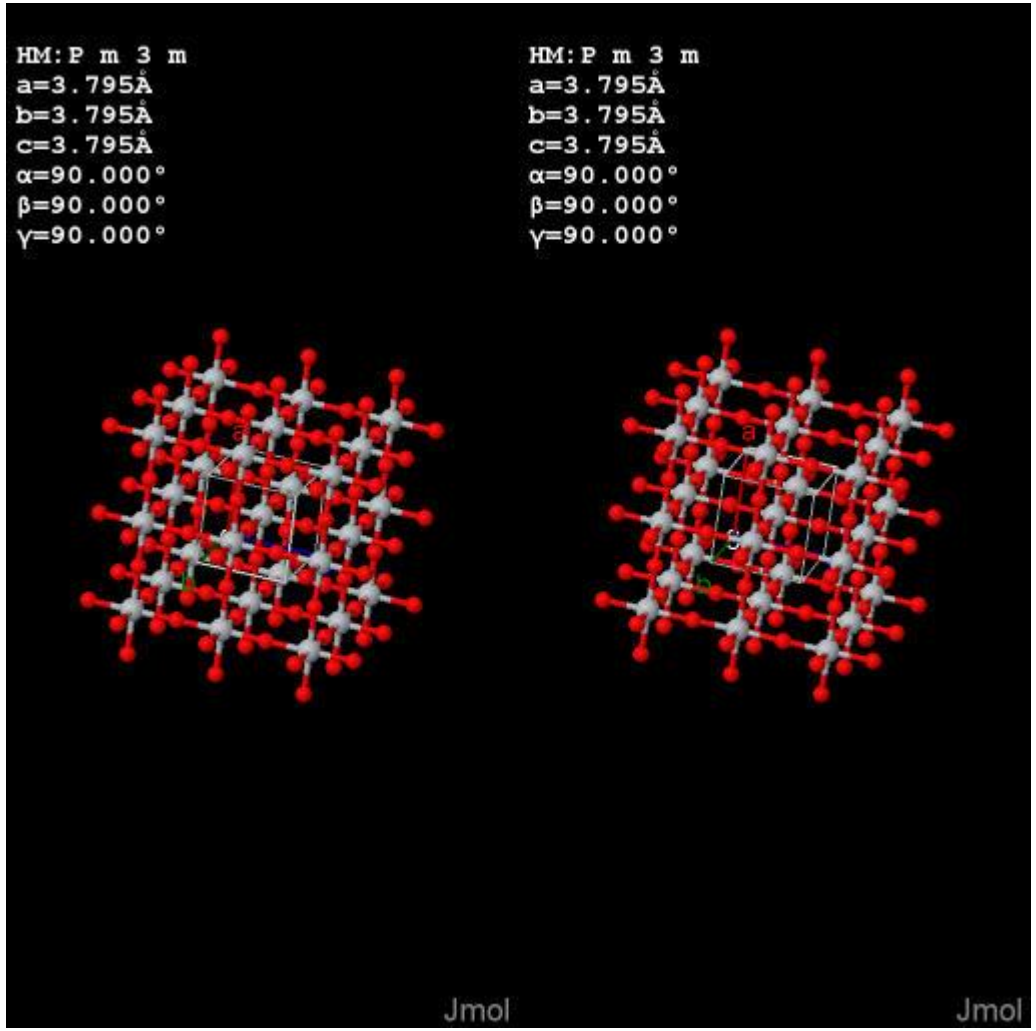
- “Magic eye view”
- Ca atoms shown… they live in the cubic gaps in between the TiO_3 framework



Barth, T. “Perovskite,” *Norsk Geologisk Tidsskrift* **1925**, *8*, 201-216.
http://rruff.geo.arizona.edu/AMS/download.php?id=18905.amc&down=amc

Cross-eyed stereogram

- Some people can see the 3D effect when they cross their eyes.
- Reading glasses help me… I find this much easier to achieve
- Ca atoms not shown



Barth, T. “Perovskite,” *Norsk Geologisk Tidsskrift* **1925**, *8*, 201-216.
http://rruff.geo.arizona.edu/AMS/download.php?id=18905.amc&down=amc

Acta Cryst E
CRYSTALLOGRAPHIC COMMUNICATIONS

Volume 70 | **Part 10** | October 2014 | Pages 178–182 | 10.1107/S1600536814019151

Crystal structures of isotypic poly[bis(benzimidazolium) [tetra-μ-iodido-stannate(II)]] and poly[bis(5,6-difluorobenzimidazolium) [tetra-μ-iodido-stannate(II)]]

I. Zimmermann, T. D. Keene, J. Hauser, S. Decurtins and S.-X. Liu

How do people approach this research?

Figure 1. The main building units of (1), showing atom labeling and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) *x*, *y* + 1, *z*; (ii) −*x*, ...

Synthetic aspect

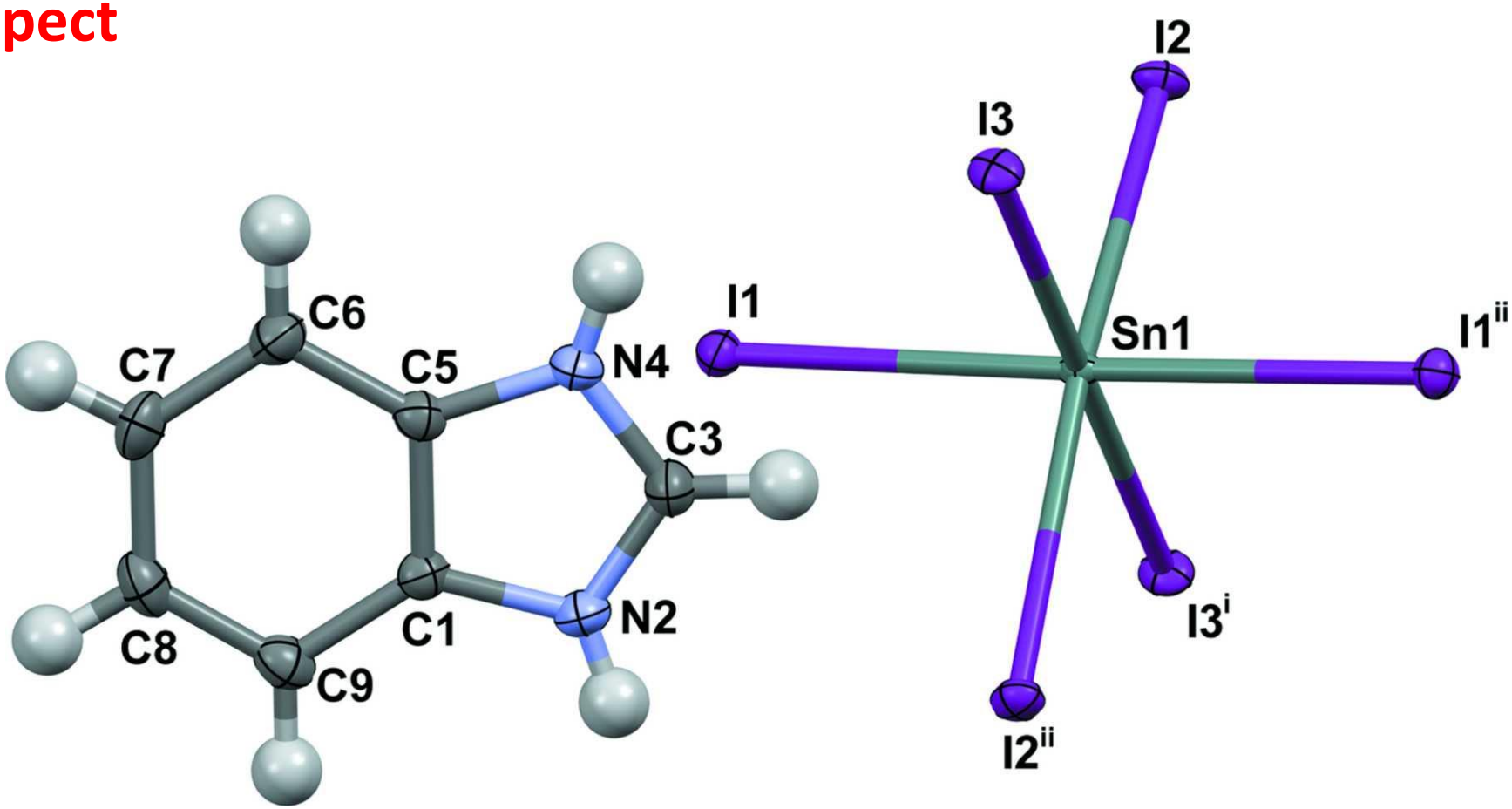


Figure 2. The main building units of (2), showing atom labeling and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) *x*, *y* + 1, *z*; (ii) −*x*, ...

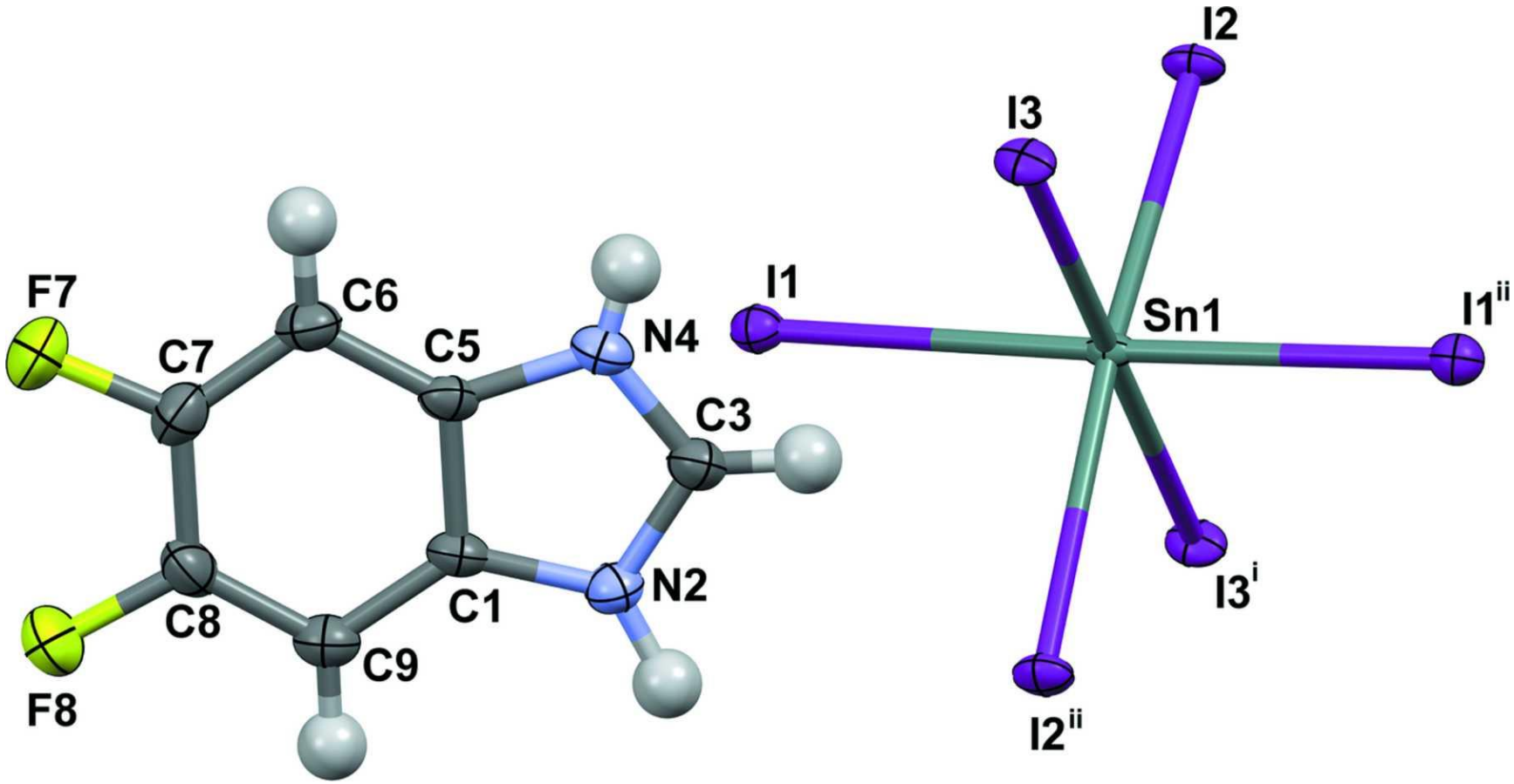


Figure 3. The crystal packing of compound (1) viewed along [010]. N—H···I hydrogen bonds are shown as dashed lines.

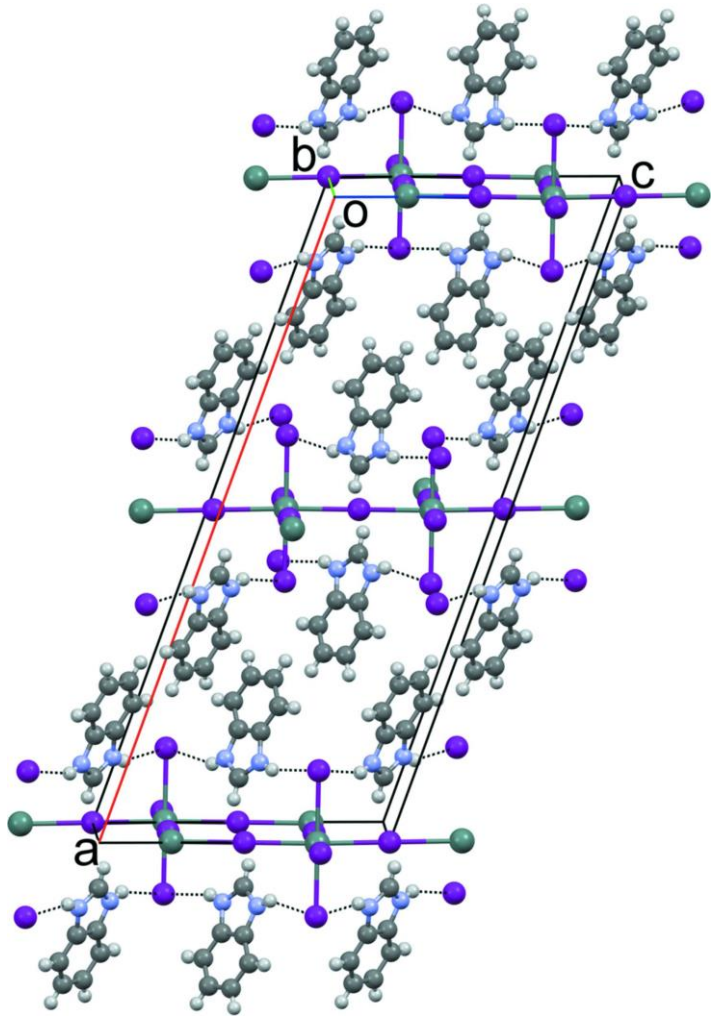
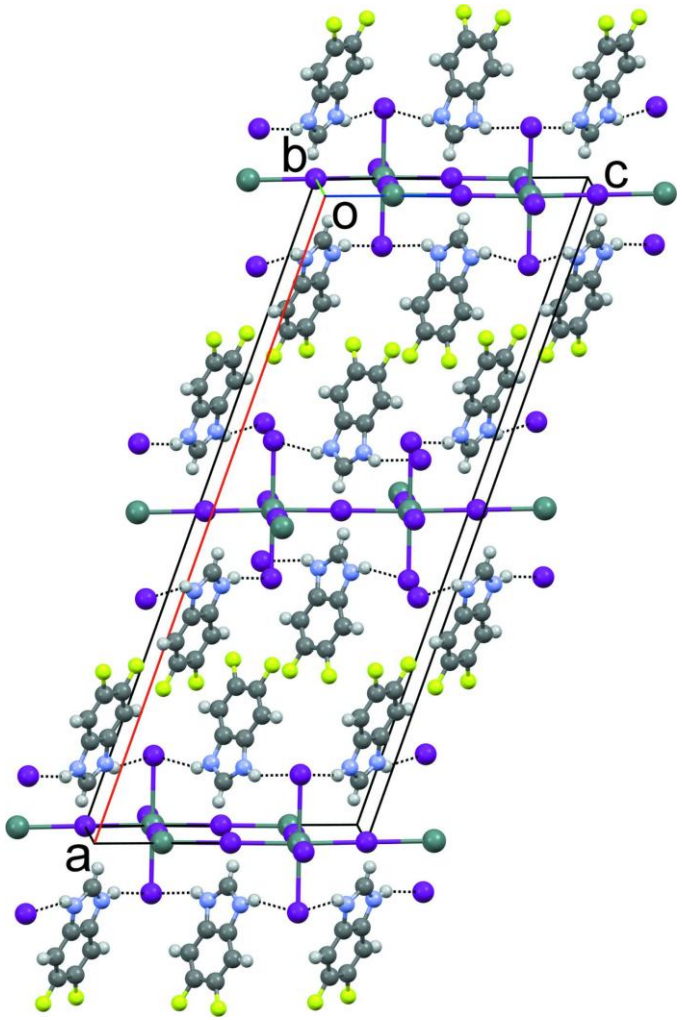


Figure 4. The crystal packing of compound (2) viewed along [010]. N—H···I hydrogen bonds are shown as dashed lines.

Distortions in structure slow down e- and hole recombinaton

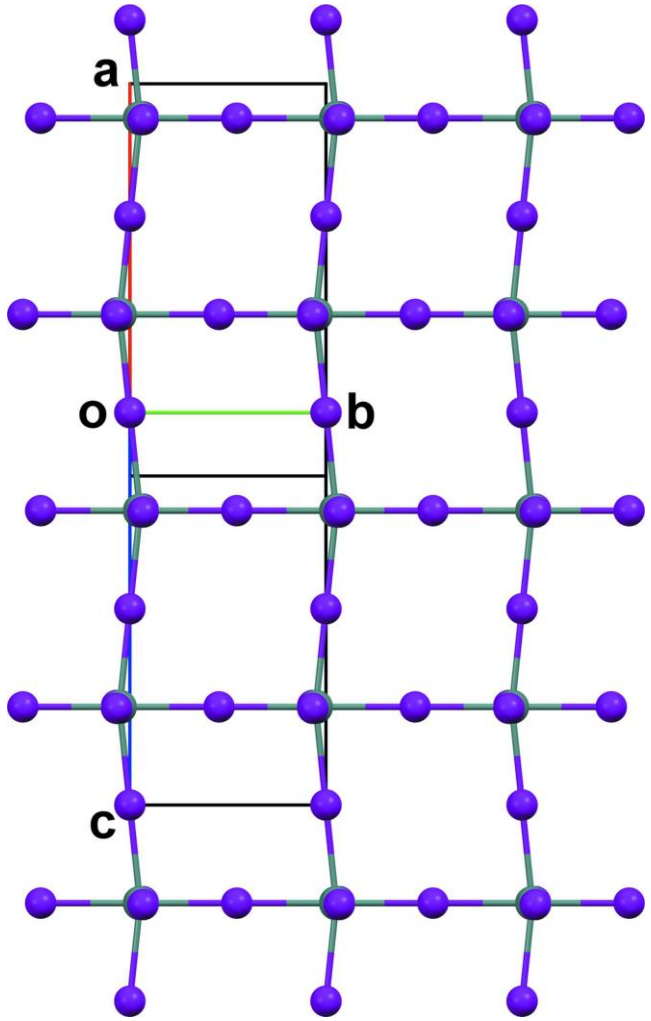


Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

Zimmermann *et al.*

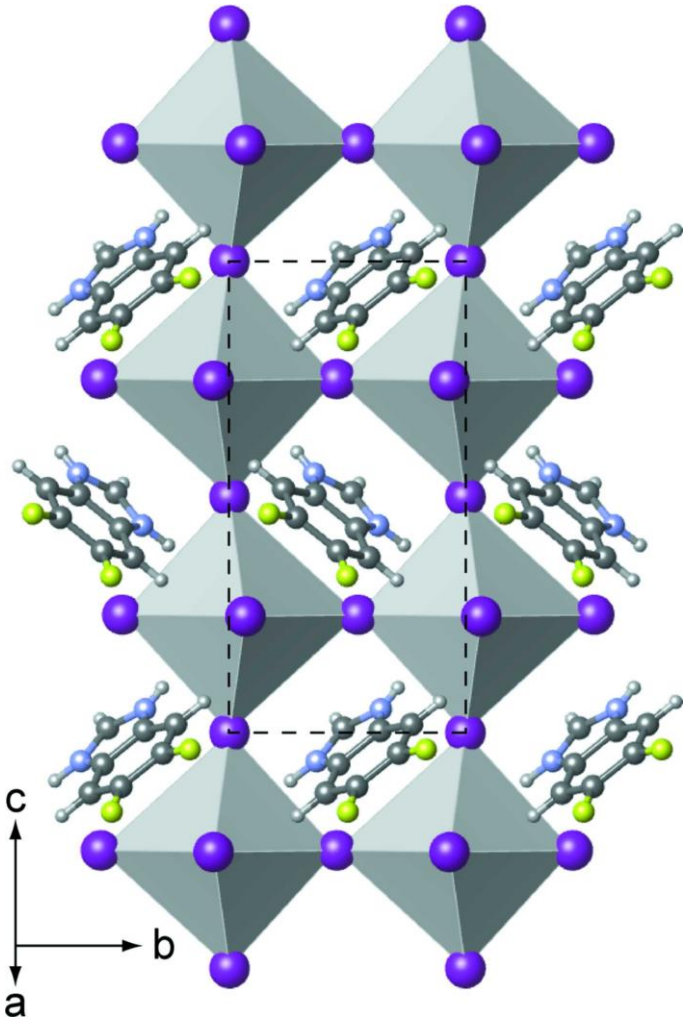
Volume 70 | **Part 10** | October 2014 | Pages 178–182 | 10.1107/S1600536814019151

Figure 5. View along the *a** axis of a tin iodide layer of (2). For clarity, the atoms are represented as spheres with uniform sizes selected for each atom type.



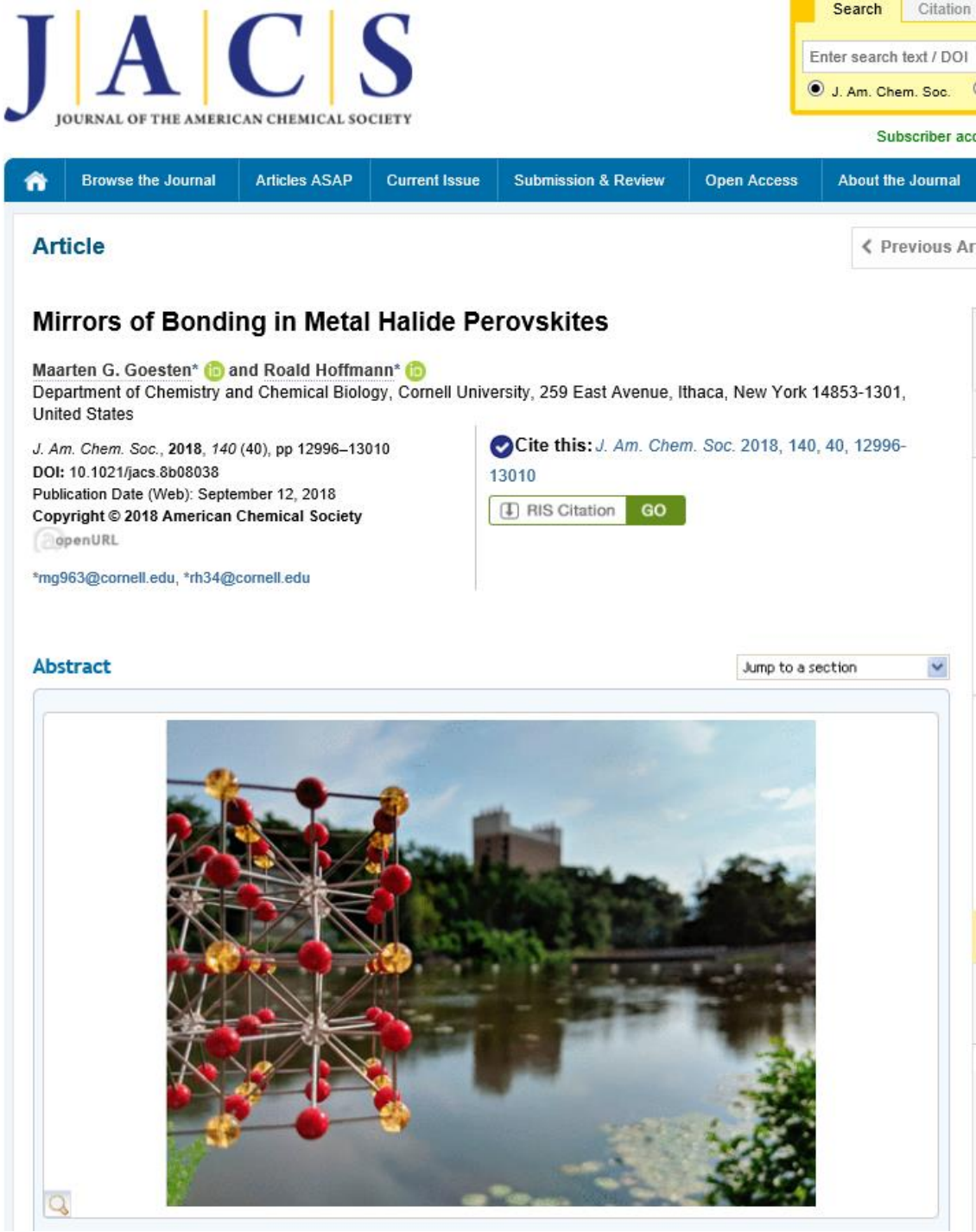
Gratuitous cat sketch

Figure 6. View along the *a** axis of a double layer of tin iodide and the organic cations of (2). For clarity, the $[SnI_6]$ octahedra are shown as polyhedra, the atoms of the organic cations ...



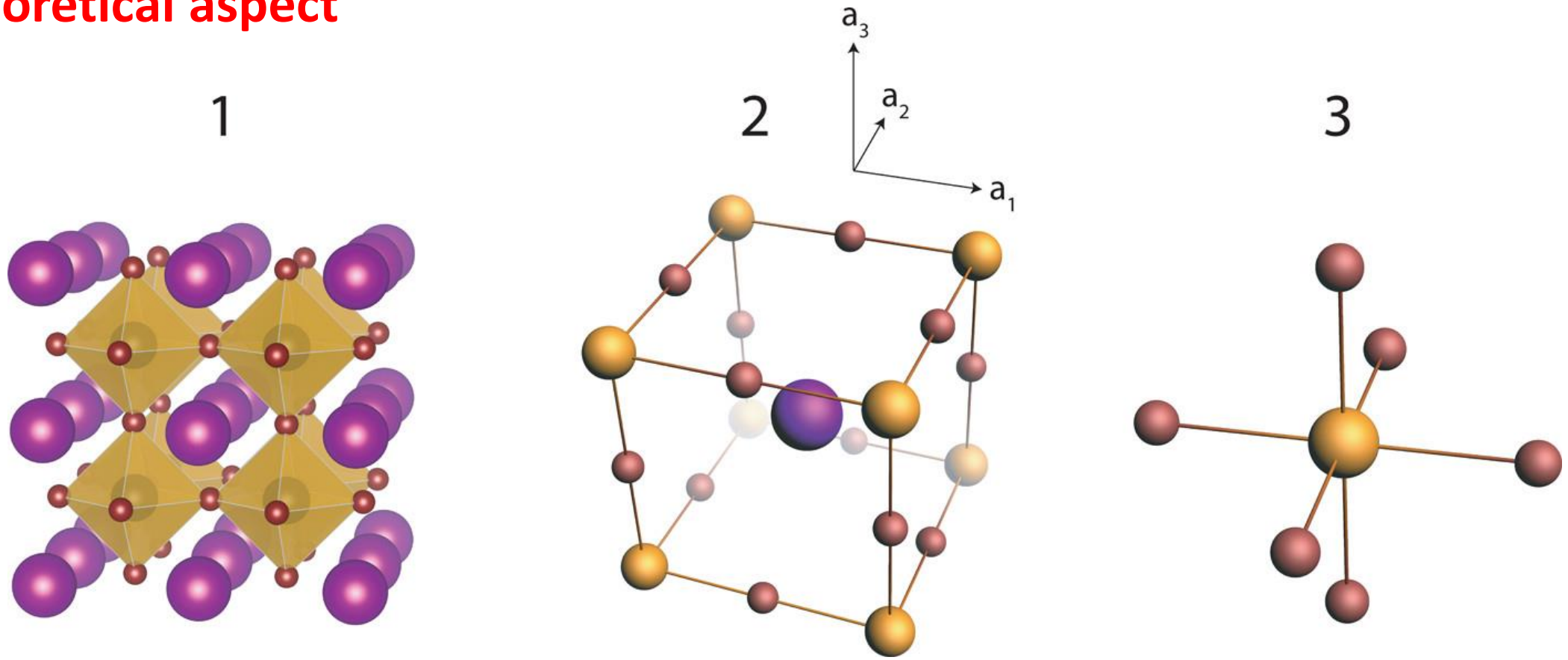
Recent Roald Hoffman Paper

- Roald Hoffman, 1981 Nobel laureate known for theoretical chemistry, which has evolved into the field of modern computational chemistry
- Also playwright, poet.
- Nice summary at
- https://en.wikipedia.org/wiki/Roald_Hoffmann



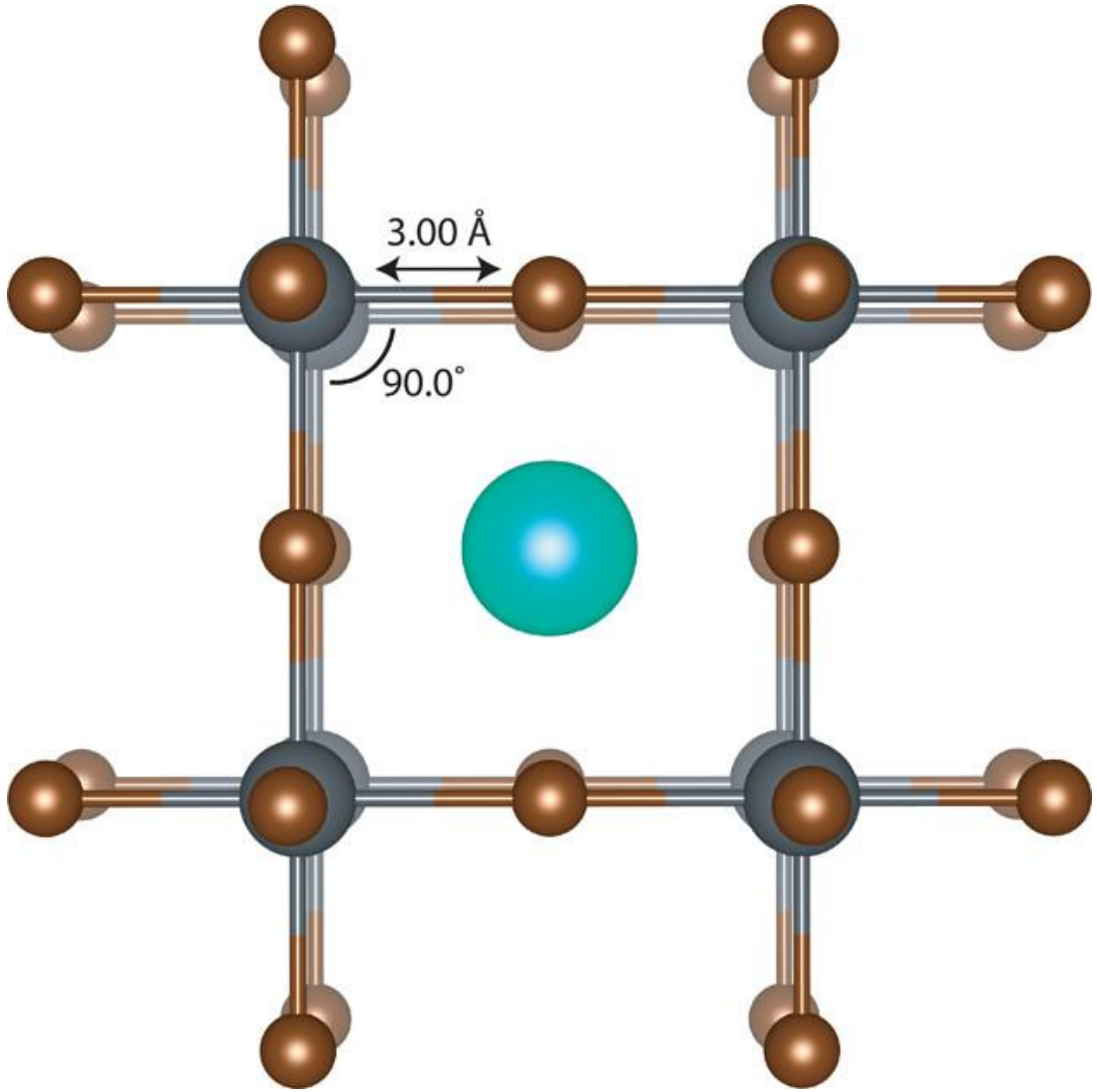
M. G. Goesten and R. Hoffmann, Mirrors of Bonding in Metal Halide Perovskites *Journal of the American Chemical Society* **2018,** *140 (40)*, 12996-13010. DOI: 10.1021/jacs.8b08038

Theoretical aspect



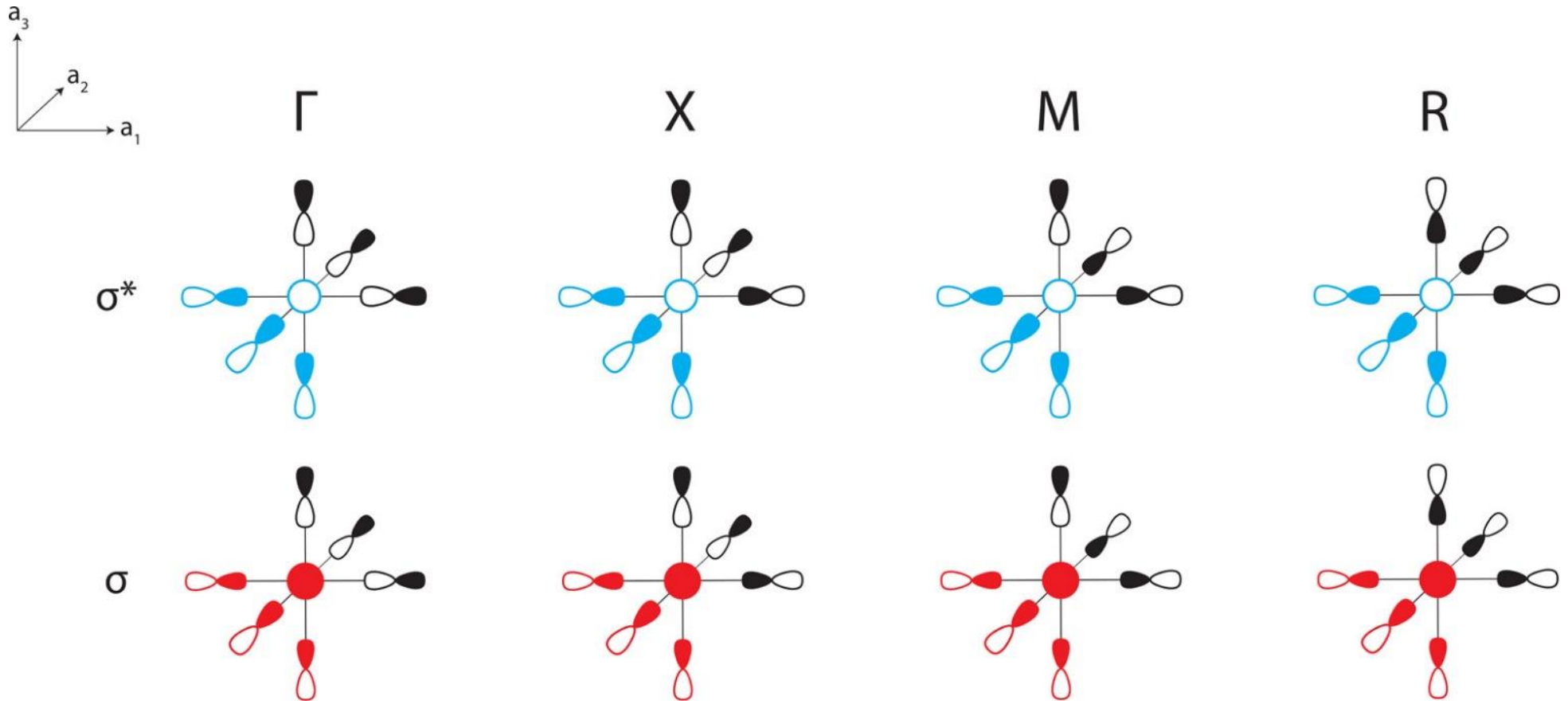
Three representations of the cubic ABX3 perovskite structure:
1, the lattice with A in purple, B as yellow octahedra, and X in burgundy;
2, primitive/conventional unit cell of ABX3; and
3, local octahedral environment around B.

Published in: Maarten G. Goesten; Roald Hoffmann; *J. Am. Chem. Soc.* 140, 12996-13010.
DOI: 10.1021/jacs.8b08038



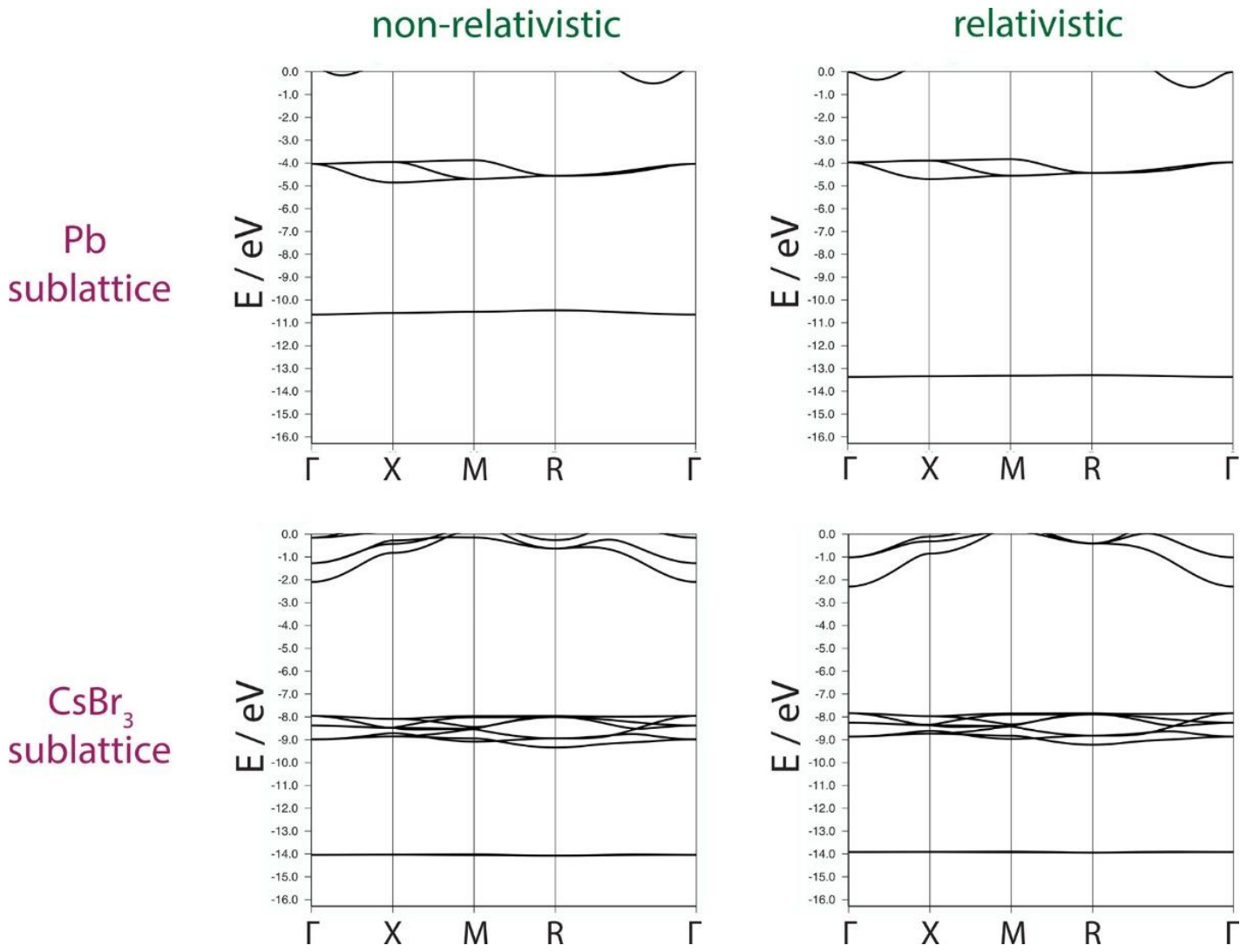
A view of the cubic structure of $CsPbBr_3$.
Color code: Pb, gray; Br, brown; Cs, turquoise.

Published in: Maarten G. Goesten; Roald Hoffmann; *J. Am. Chem. Soc.* 140, 12996-13010.
DOI: 10.1021/jacs.8b08038



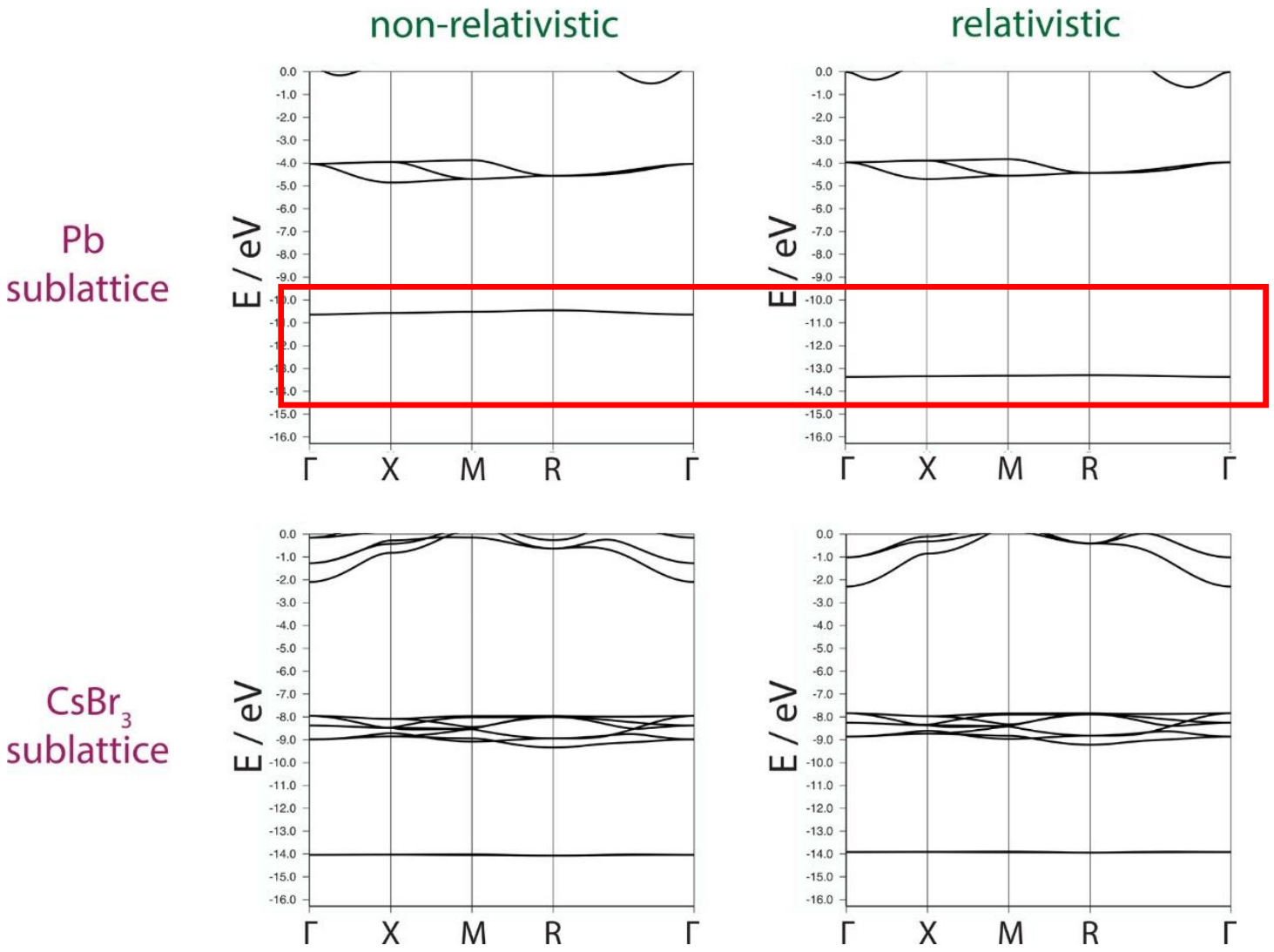
σ and σ* crystal orbitals along Γ-X-M-R, represented by a $PbBr_6$ octahedral unit. The orbital bases for the σ and σ* bands are colored red and blue, respectively.

Published in: Maarten G. Goesten; Roald Hoffmann; *J. Am. Chem. Soc.* 140, 12996-13010.
DOI: 10.1021/jacs.8b08038



Computed band structures of the Pb and $CsBr_3$ sublattices in $CsPbBr_3$.

Published in: Maarten G. Goesten; Roald Hoffmann; *J. Am. Chem. Soc.* 140, 12996-13010.
DOI: 10.1021/jacs.8b08038



Details are way beyond the scope of this talk… (also beyond my current ability to articulate)

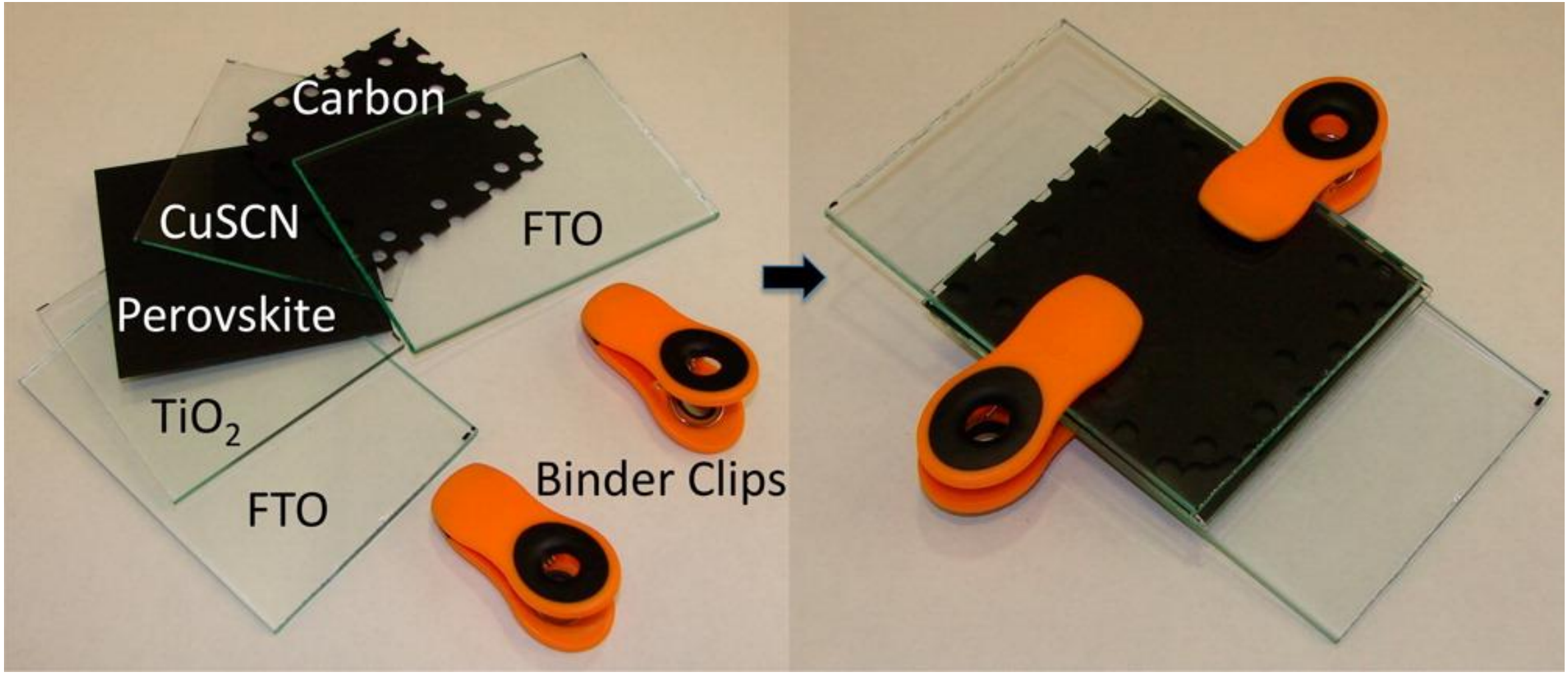
Major point: s-electrons in heavy elements move at a significant fraction of the speed of light when they get close to the nucleus

… enough so mass changes need to be taken into account for accurate calculations.

… need relativistic effects to correctly predict yellow color for gold.

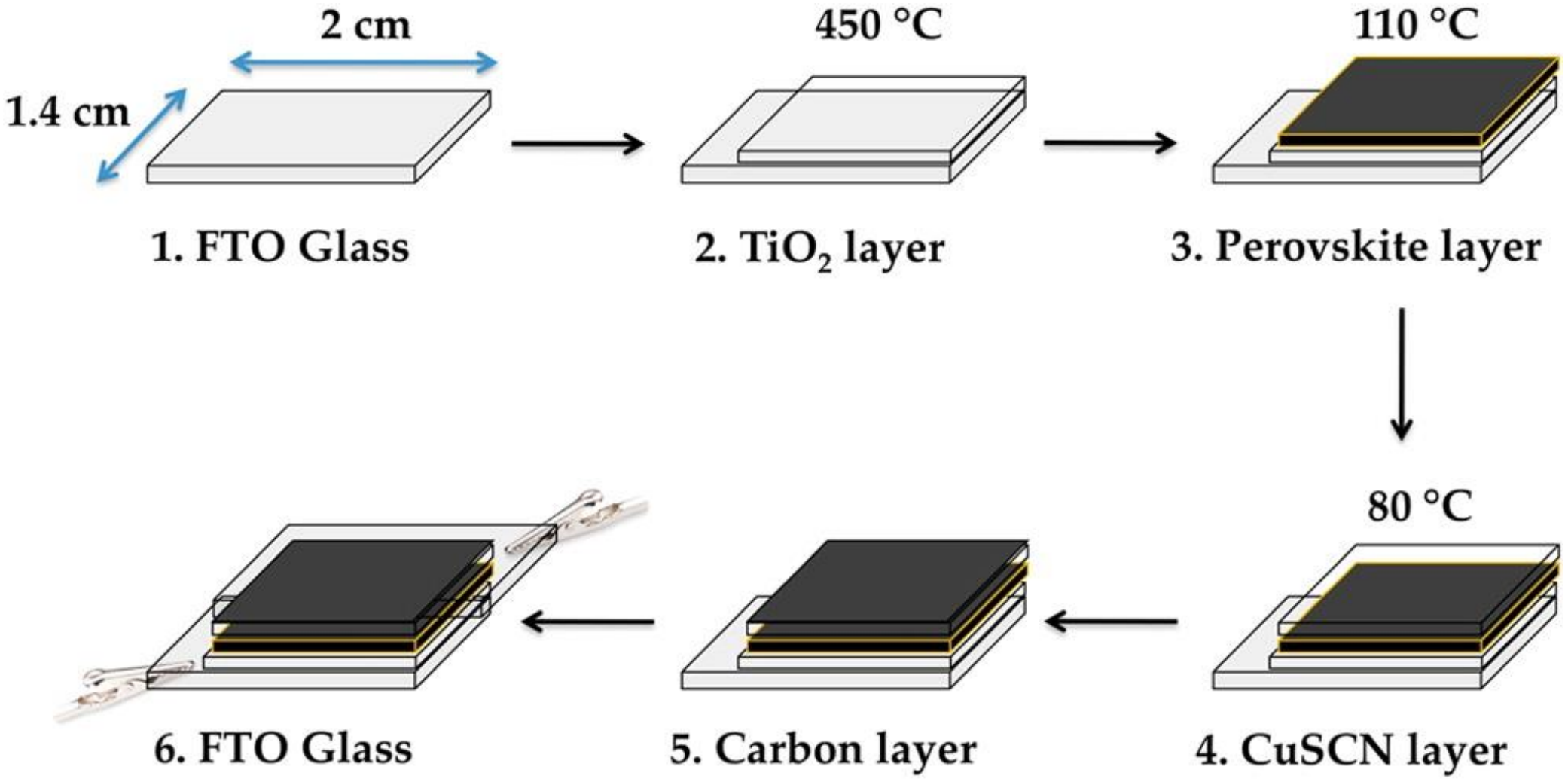
Computed band structures of the Pb and $CsBr_3$ sublattices in $CsPbBr_3$.

Published in: Maarten G. Goesten; Roald Hoffmann; *J. Am. Chem. Soc.* 140, 12996-13010.
DOI: 10.1021/jacs.8b08038



A physical model that is appropriate to teach the design and fabrication of perovskite solar cell in classrooms.

Published in: Sameer Patwardhan; Duyen H. Cao; Shelby Hatch; Omar K. Farha; Joseph T. Hupp; Mercouri G. Kanatzidis; George C. Schatz; *J. Phys. Chem. Lett.* **2015,** 6, 251-255. DOI: 10.1021/jz502648y



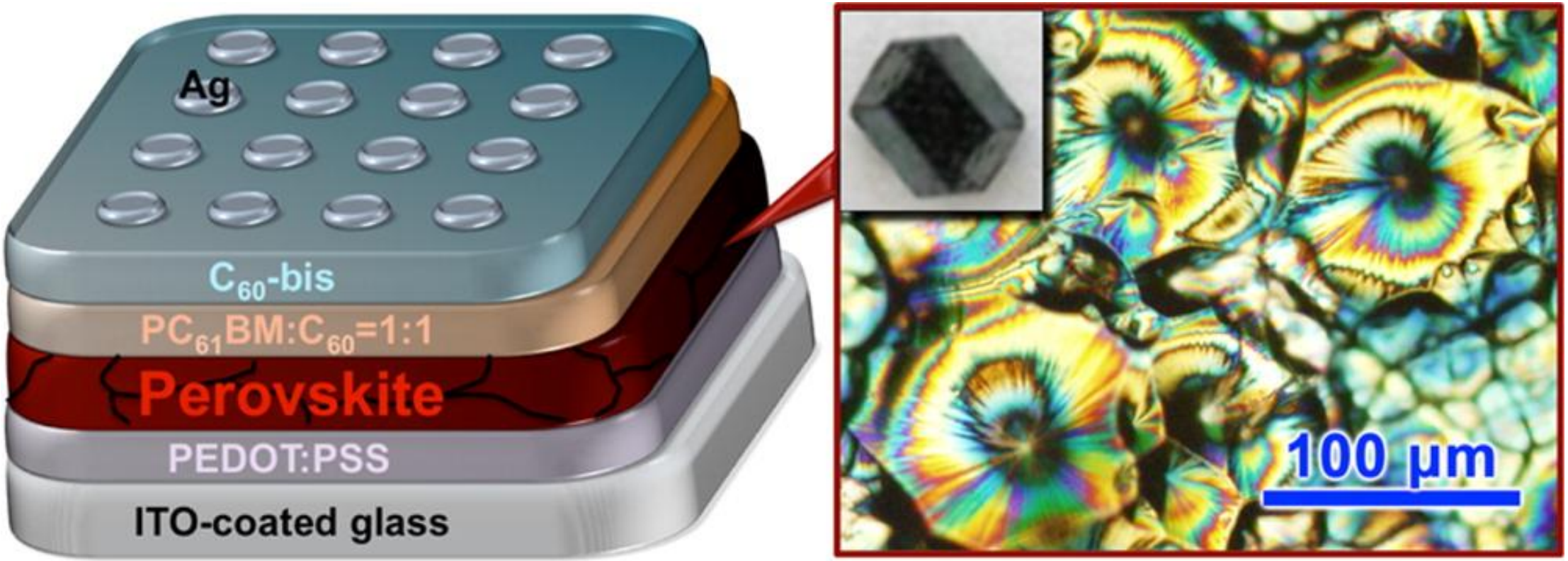
Fabrication procedure for perovskite solar cells.

Published in: Sameer Patwardhan; Duyen H. Cao; Shelby Hatch; Omar K. Farha; Joseph T. Hupp; Mercouri G. Kanatzidis; George C. Schatz; *J. Phys. Chem. Lett.* **2015,** 6, 251-255. DOI: 10.1021/jz502648y

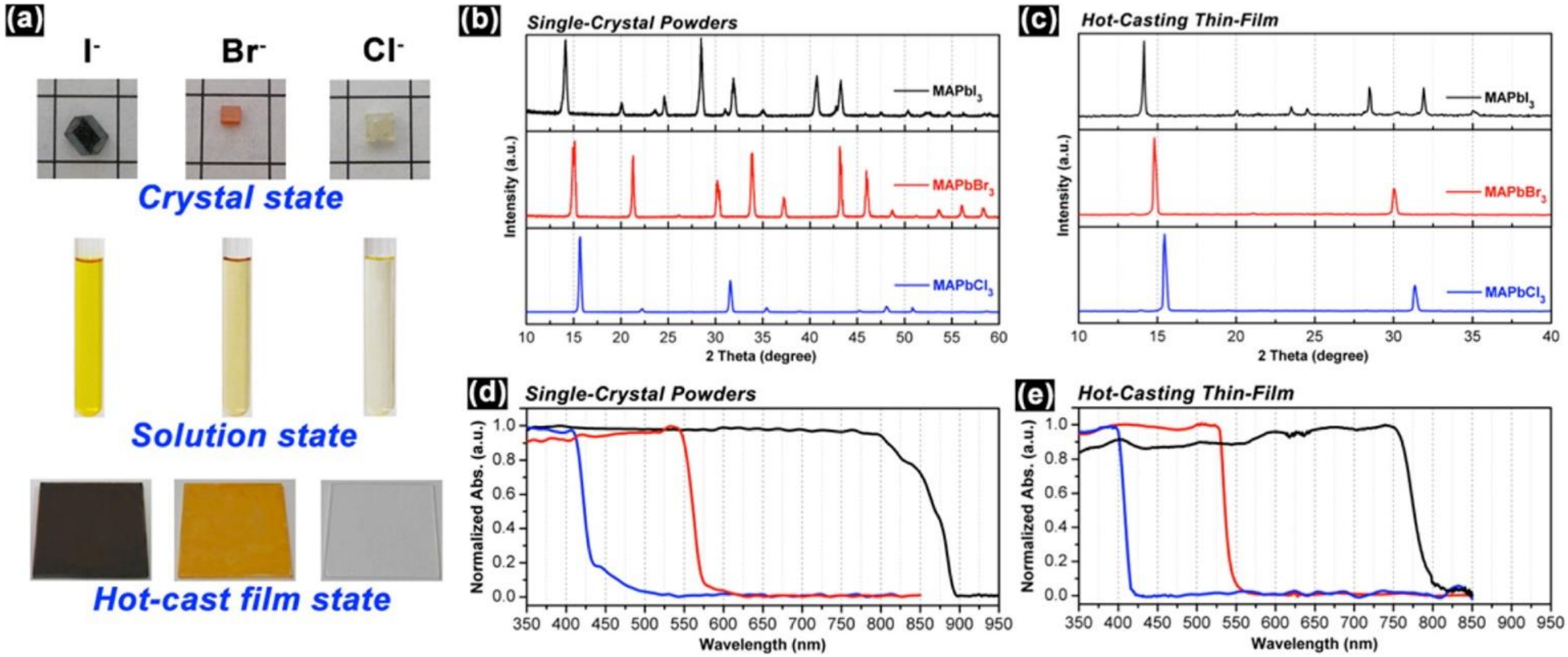
Measurement of the photovoltage under sunlight and in dark conditions.
The device is kept in the palm of one hand, controlling the exposure to sunlight with the other.

Published in: Sameer Patwardhan; Duyen H. Cao; Shelby Hatch; Omar K. Farha; Joseph T. Hupp; Mercouri G. Kanatzidis; George C. Schatz;
J. Phys. Chem. Lett. **2015,** 6, 251-255.DOI: 10.1021/jz502648y

Large grain perovskite solar cells



Published in: Hung-Ju Yen; Po-Wei Liang; Chu-Chen Chueh; Zhibin Yang; Alex K.-Y. Jen; Hsing-Lin Wang;
ACS Appl. Mater. Interfaces **2016,** 8, 14513-14520.
DOI: 10.1021/acsami.6b02169.



(a) Photographs of three perovskite materials ($MAPbX_3$, X = I^-, Br^-, or Cl^-) as solution, crystal, and hot-cast film states.
(b) (b, c) XRD spectra of single-crystal powders and hot-cast thin films.
(c) (d, e) UV–vis absorption spectra of three perovskite materials as crystal and hot-cast film states.

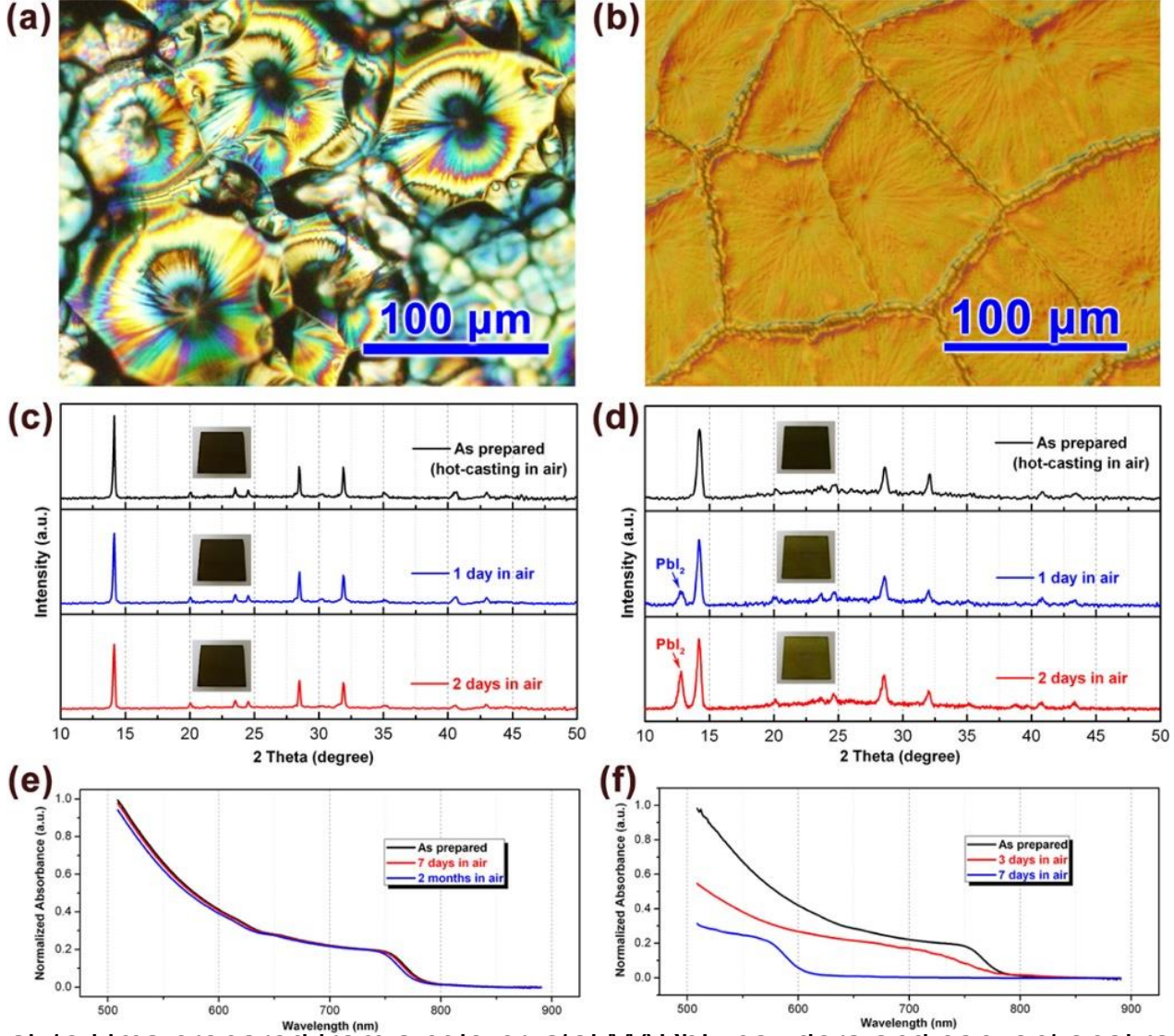
Published in: Hung-Ju Yen; Po-Wei Liang; Chu-Chen Chueh; Zhibin Yang; Alex K.-Y. Jen; Hsing-Lin Wang; *ACS Appl. Mater. Interfaces* **2016,** 8, 14513-14520.
DOI: 10.1021/acsami.6b02169

This side:

Single crystalline Materials. Means high purity

This side:

In-situ prep Poorly crystalline!



Sharp X-Ray signals

Broad X-Ray signals PbI_2 impurity

Long lasting!

Quickly degrades!

(a, b) Optical micrographs of the perovskite films prepared from single-crystal $MAPbI_3$ powders and conventional route (MAI + PbI2) via hot-casting method.
(c, d) XRD spectra of perovskite; inset images are the photographs of the corresponding films.
(e, f) UV–vis of perovskite films on PEDOT:PSS substrates prepared from $MAPbI_3$ single crystals and conventional route (MAI + PbI_2) as a function of storage time in ambient condition (25 ° C, 55% relative humidity).

Published in: Hung-Ju Yen; Po-Wei Liang; Chu-Chen Chueh; Zhibin Yang; Alex K.-Y. Jen; Hsing-Lin Wang;
ACS Appl. Mater. Interfaces **2016,** 8, 14513-14520.
DOI: 10.1021/acsami.6b02169.

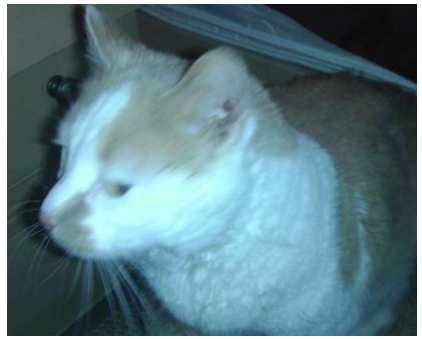
Some conclusions

- New tricks from a common structure…
- Extremely rapid progress over a decade, compared to next best material (doped silicon)
- Potential for further improvements to stability, and efficiency
- Potential for further development for LED applications

Some resources

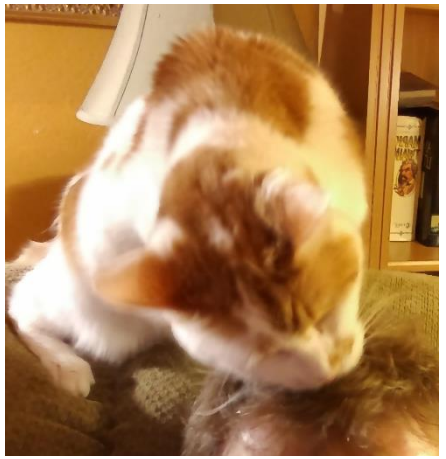
- “JMOL: an open-source Java viewer for chemical structures in 3D”
  - http://jmol.sourceforge.net/
- Data repositories:
  - Crystallography Open Database
  - Research Collaboratory for Structural Bioinformatics
  - http://www.crystallography.net/cod/index.php
  - http://rruff.geo.arizona.edu/AMS/amcsd.php
- Blender:
  - https://www.blender.org/

Thanks!

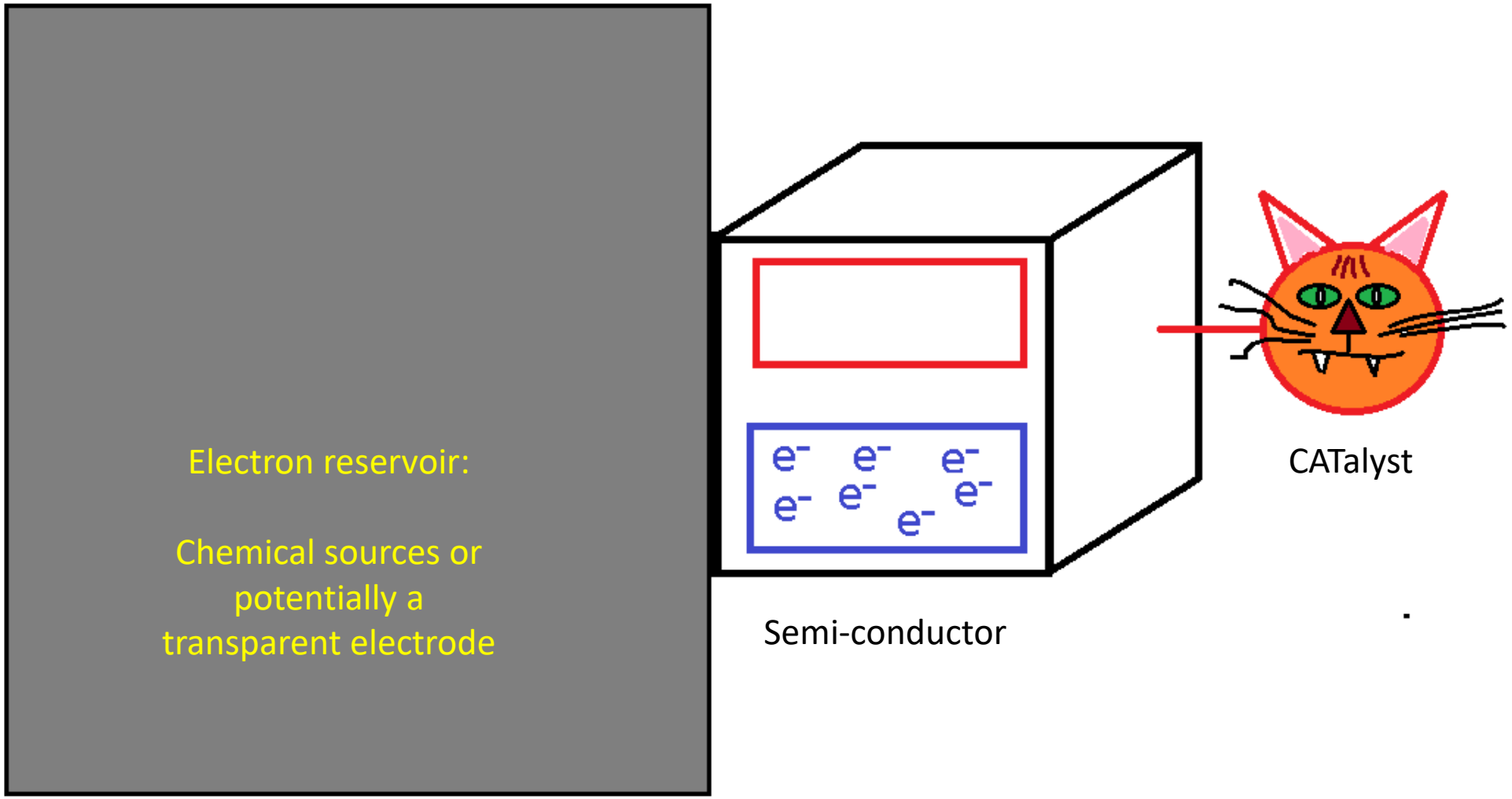


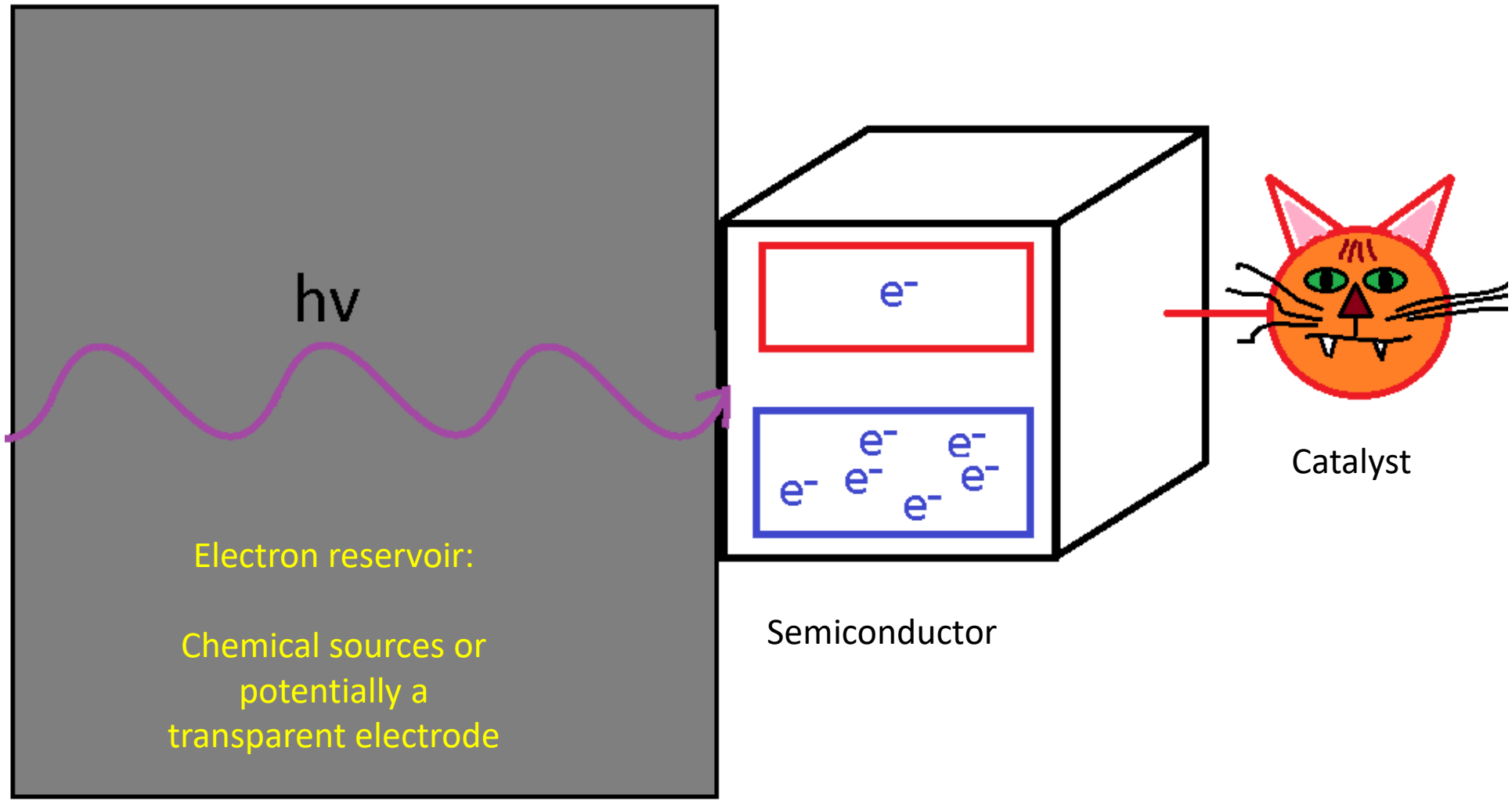
- Members and Students of the Science Circle!
- Students and Faculty of Dept. of Chem., SIUE.
- Generous support of National Science Foundation for our work on heme-nitrosyl complexes, NSF-CHE 1566509
- DPA-LLC for hosting animated gifs and other files on their website

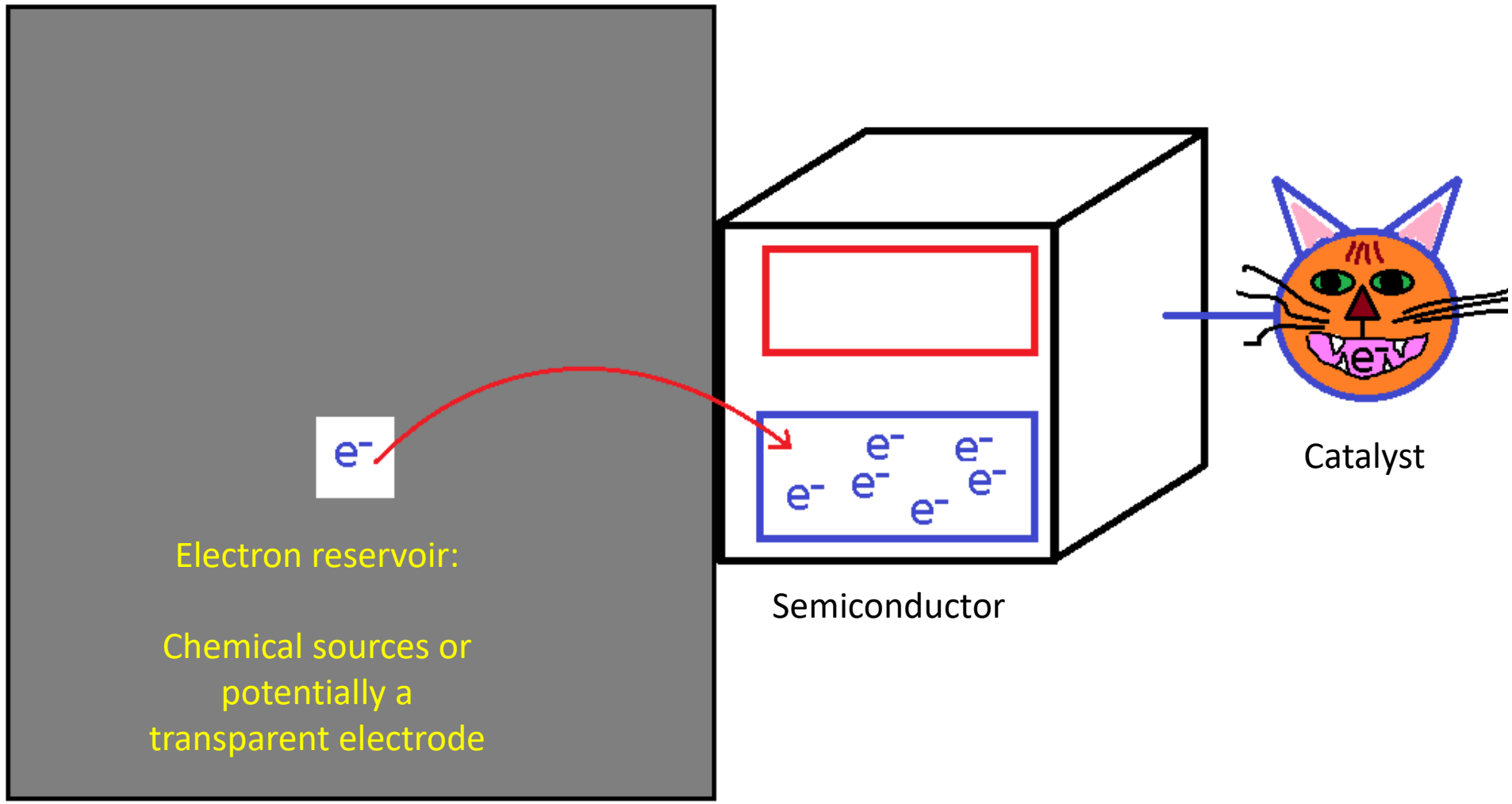
- My cats for their patience…



Dye-sensitized solar cell




hv
e⁻
e⁻ e⁻ e⁻ e⁻ e⁻
Electron reservoir:
Chemical sources or potentially a transparent electrode
Semiconductor
Catalyst


e⁻
Electron reservoir:
Chemical sources or
potentially a
transparent electrode
e⁻ e⁻ e⁻ e⁻ e⁻
Semiconductor
Catalyst

Action of Catalyst